

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080222\
 Data File : BM036068.D
 Acq On : 03 Aug 2022 01:09
 Operator : CG/JU
 Sample : N3896-11
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RVE-68

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036068.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.434	392	399	407	rBV	5841154	8322246	8.38%	3.260%
2	7.039	662	672	686	rBV	5719967	8959104	9.02%	3.509%
3	7.869	803	813	820	rBV	1157219	1859681	1.87%	0.728%
4	9.039	1003	1012	1019	rBV	3503643	5714518	5.76%	2.238%
5	10.675	1280	1290	1295	rBV	1650745	2821270	2.84%	1.105%
6	13.133	1699	1708	1722	rBV	9274584	13364826	13.46%	5.235%
7	14.504	1932	1941	1948	rBV	2557591	3751395	3.78%	1.469%
8	15.992	2187	2194	2202	rBV	7558124	10627692	10.70%	4.163%
9	17.245	2401	2407	2412	rBV	3286662	4532977	4.57%	1.776%
10	18.150	2554	2561	2570	rVB2	1823239	2826233	2.85%	1.107%
11	19.303	2749	2757	2764	rBV	1570056	2669015	2.69%	1.045%
12	19.662	2810	2818	2827	rVB	977616	1670914	1.68%	0.655%
13	19.874	2848	2854	2859	rBV	17487849	21241368	21.39%	8.321%
14	21.139	3065	3069	3076	rBV	3110505	3905498	3.93%	1.530%
15	21.421	3111	3117	3121	rBV	4369621	6076550	6.12%	2.380%
16	22.056	3223	3225	3230	rVB	814585	1065243	1.07%	0.417%
17	22.774	3342	3347	3358	rVB	1274674	1932723	1.95%	0.757%
18	23.068	3392	3397	3402	rBV	1171923	2136140	2.15%	0.837%
19	23.127	3403	3407	3418	rVB3	1006719	1888432	1.90%	0.740%
20	23.785	3513	3519	3526	rBV2	2126090	4033048	4.06%	1.580%
21	24.032	3557	3561	3570	rVB	689829	1302894	1.31%	0.510%
22	24.409	3620	3625	3634	rVB	828570	1726938	1.74%	0.676%
23	24.509	3637	3642	3653	rVB	695607	1583024	1.59%	0.620%
24	25.738	3847	3851	3859	rVB2	634943	1462727	1.47%	0.573%
25	26.232	3928	3935	3948	rVB5	1068688	3456876	3.48%	1.354%
26	26.544	3971	3988	4002	rVB2	25780958	99289819	100.00%	38.893%
27	26.709	4009	4016	4025	rVB	1385137	3812676	3.84%	1.493%
28	27.079	4069	4079	4088	rBV2	5607946	16749380	16.87%	6.561%
29	27.915	4210	4221	4234	rVB2	4740085	16503448	16.62%	6.465%

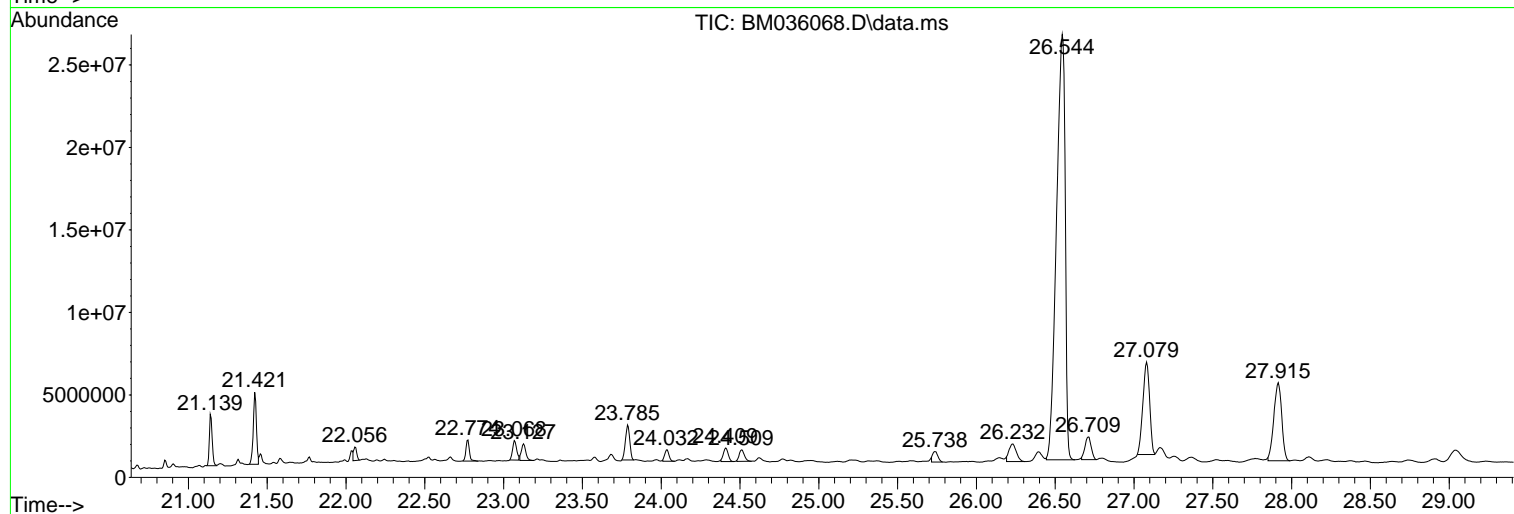
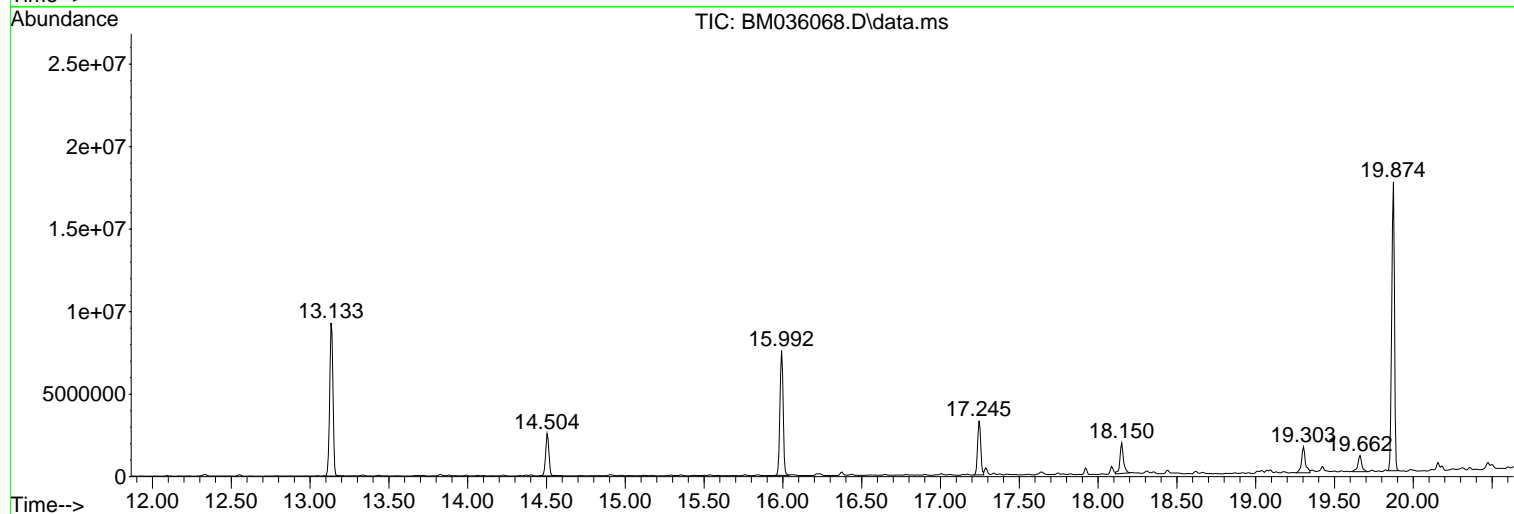
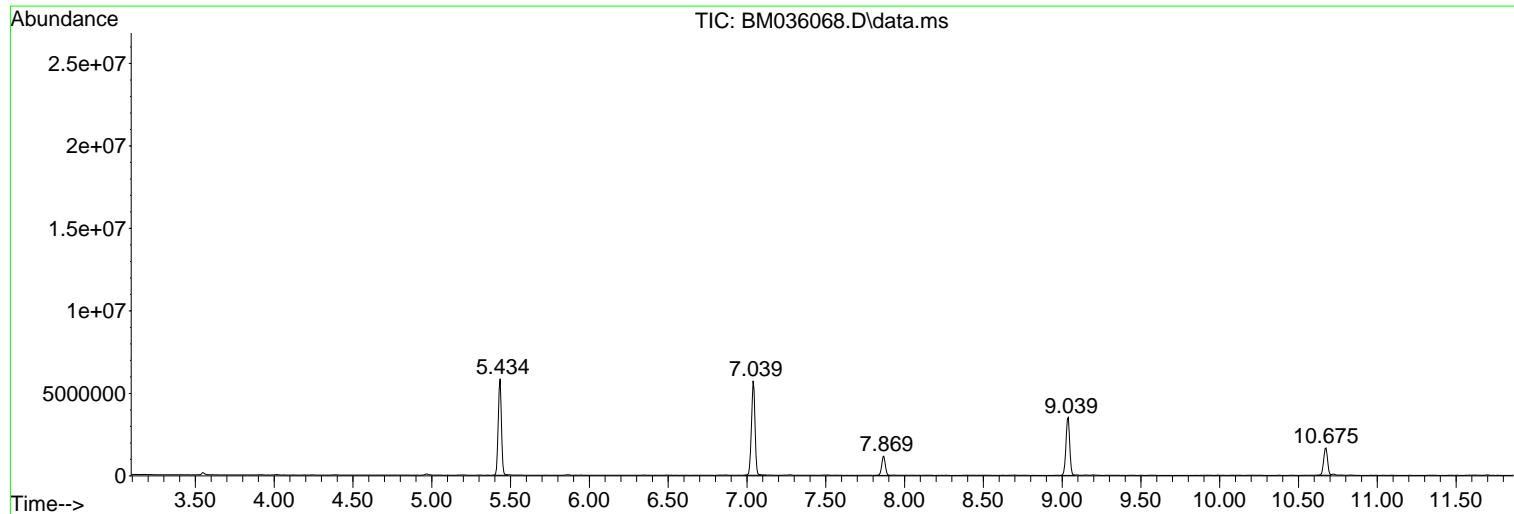
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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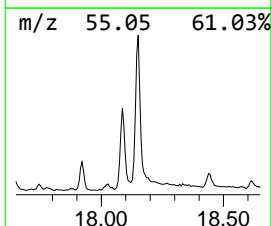
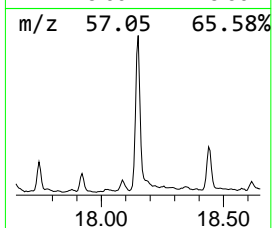
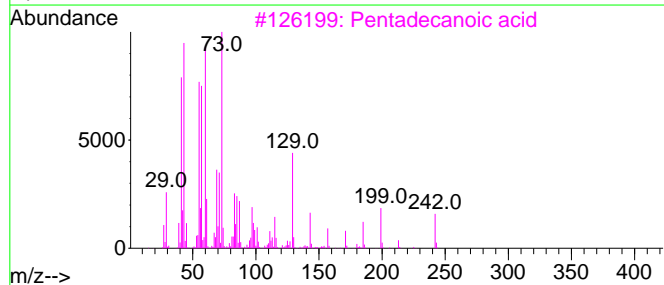
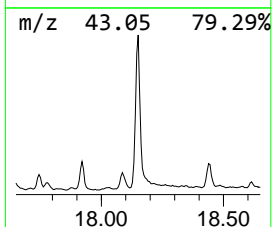
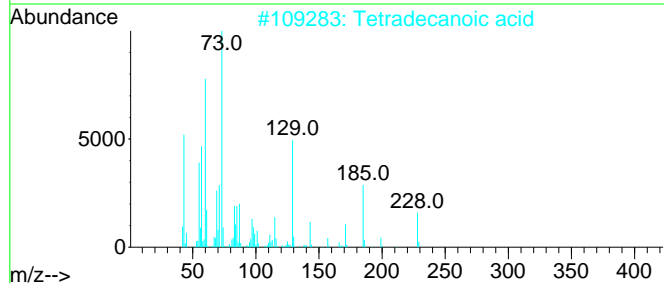
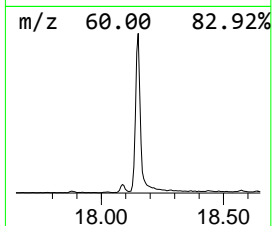
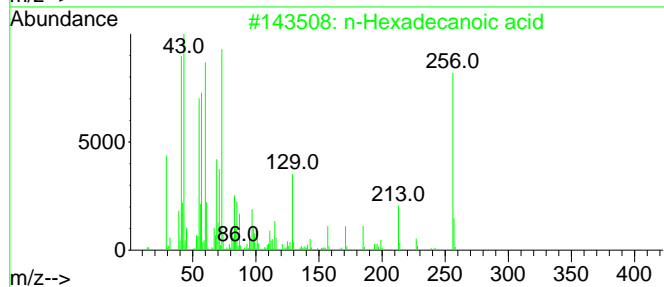
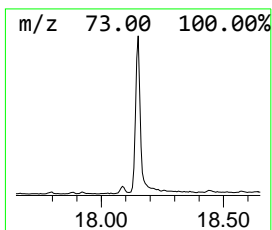
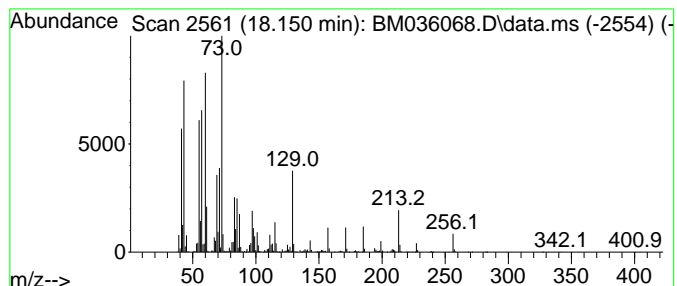
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 Peak Number 1 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	12.47 ng	2826230	Phenanthrene-d10	17.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tridecanoic acid	214	C13H26O2	000638-53-9	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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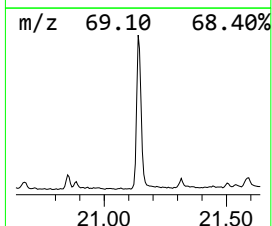
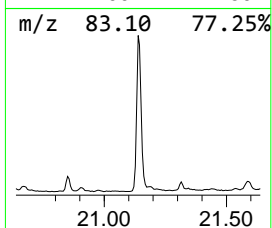
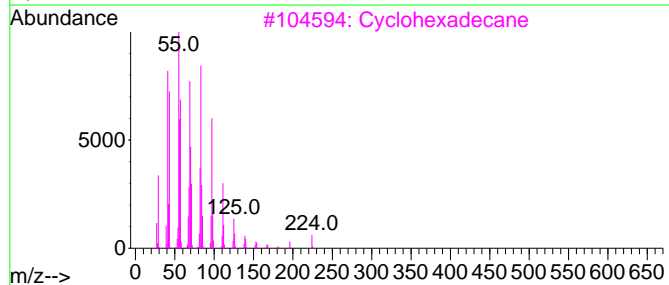
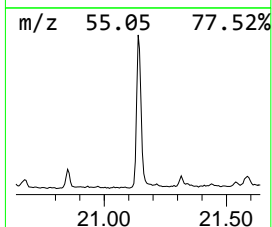
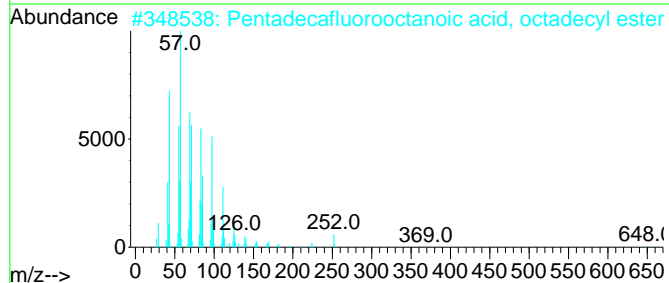
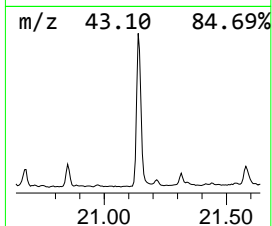
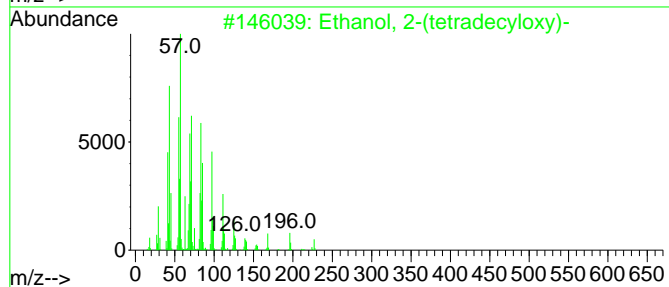
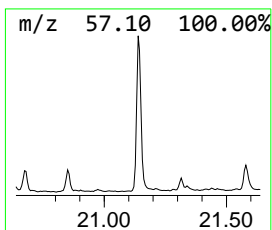
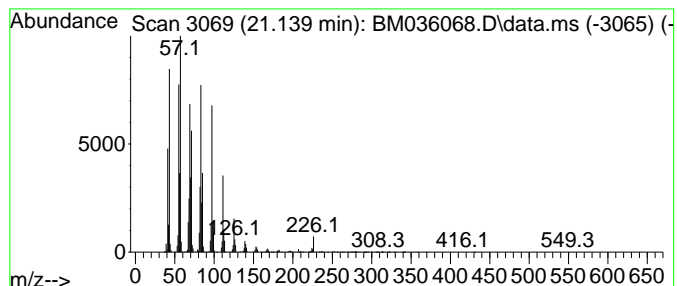
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 Peak Number 2 Ethanol, 2-(tetradecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.139	12.85 ng	3905500	Chrysene-d12	21.421

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	98
2		Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
3		Cyclohexadecane	224	C16H32	000295-65-8	94
4		1-Hexacosene	364	C26H52	018835-33-1	94
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



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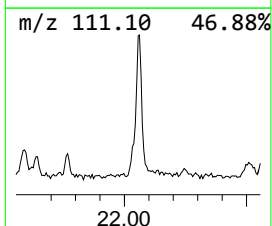
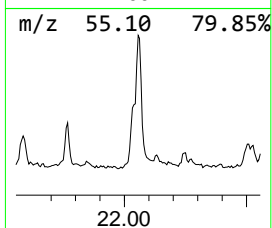
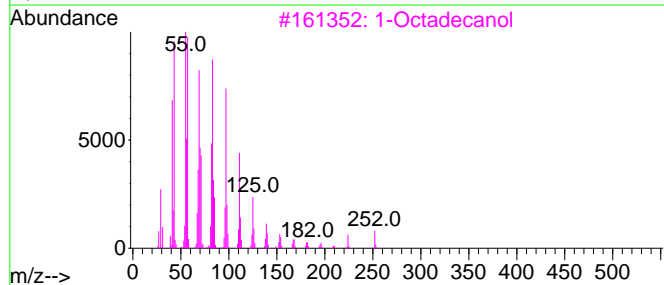
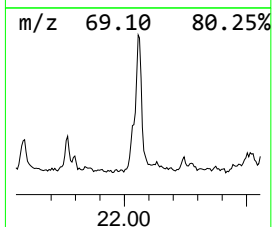
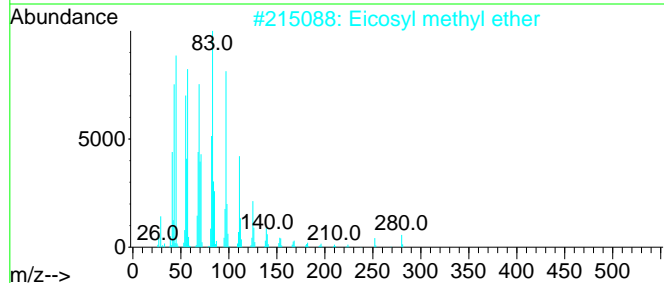
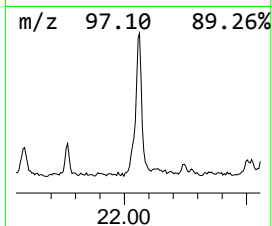
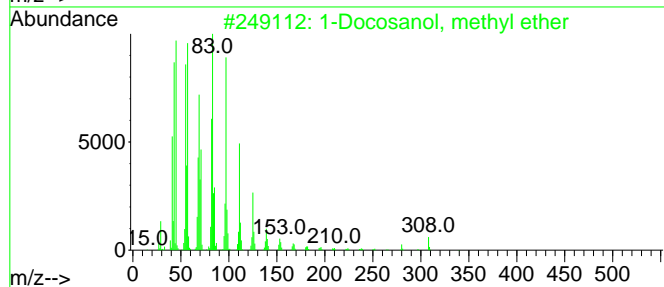
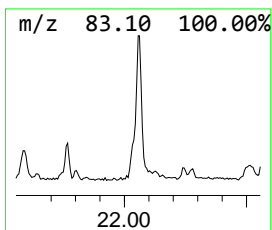
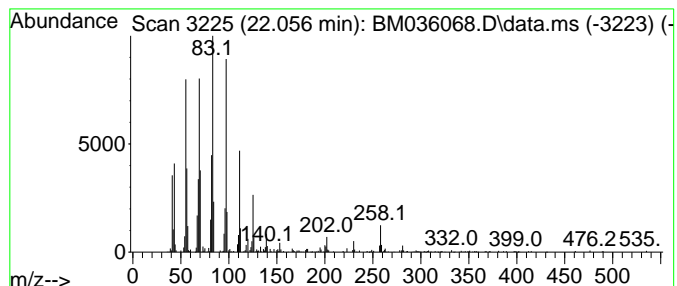
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TIC Library : C:\Database\NIST20.L
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 Peak Number 3 1-Docosanol, methyl ether Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	3.51 ng	1065240	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	94
2			Eicosyl methyl ether	312	C21H44O	1000406-29-4	91
3			1-Octadecanol	270	C18H38O	000112-92-5	76
4			Octacosanol	410	C28H58O	000557-61-9	74
5			Fumaric acid, 2-chloroethyl octa...	430	C24H43ClO4	1000330-62-4	72



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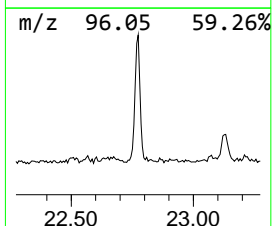
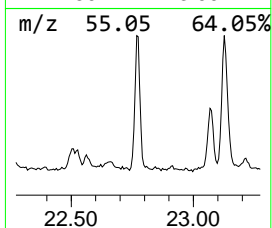
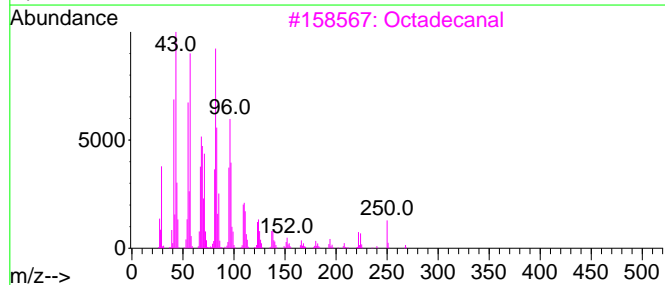
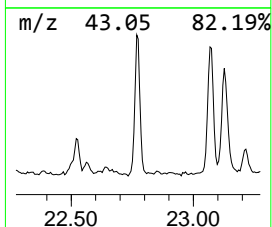
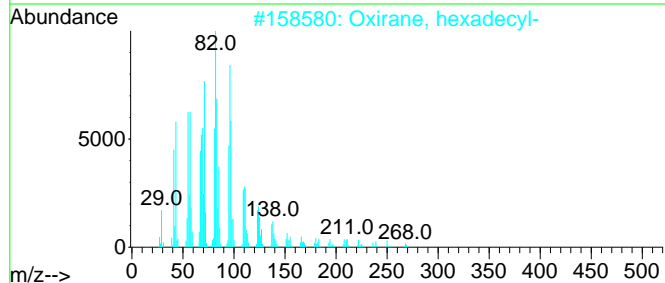
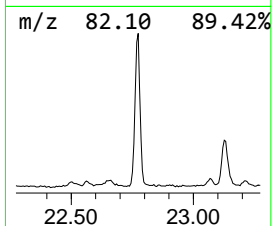
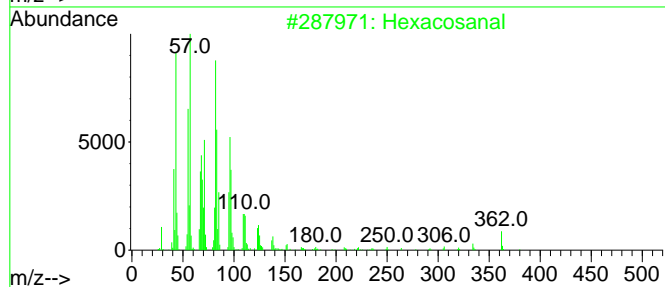
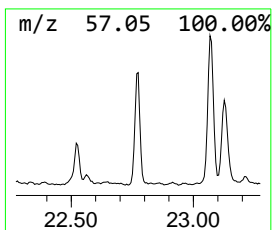
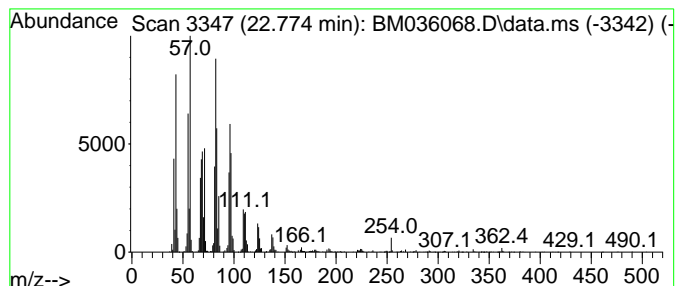
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 Peak Number 4 Hexacosanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.774	9.58 ng	1932720	Perylene-d12	23.785

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosanal	380	C26H52O	026627-85-0	96
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	95
3		Octadecanal	268	C18H36O	000638-66-4	95
4		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
5		Nonacosanal	422	C29H58O	072934-04-4	94



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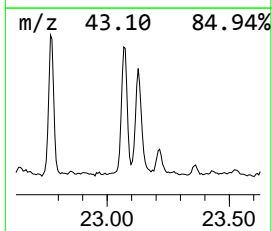
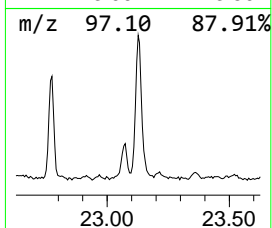
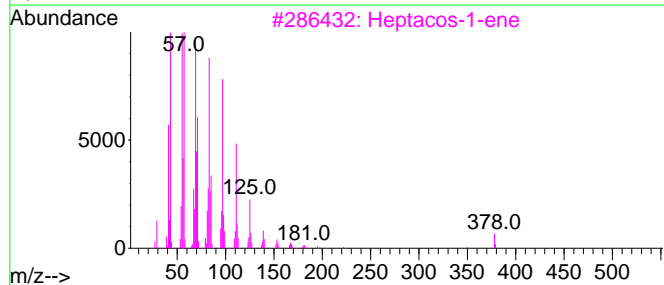
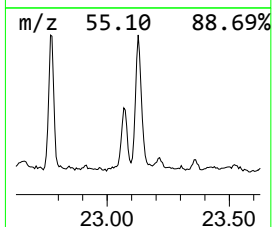
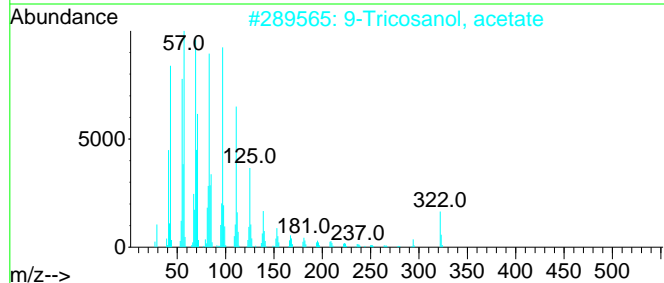
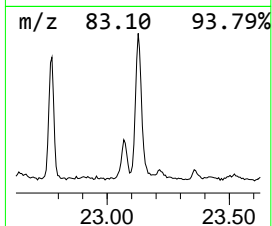
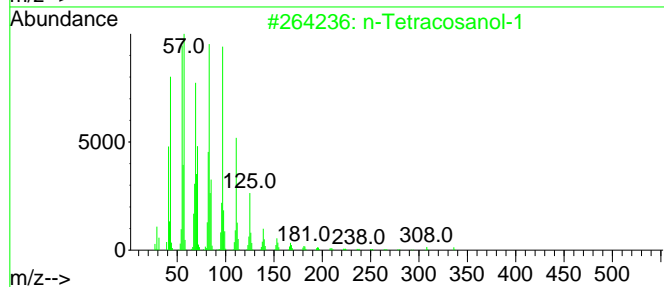
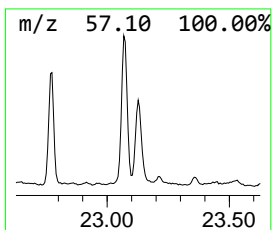
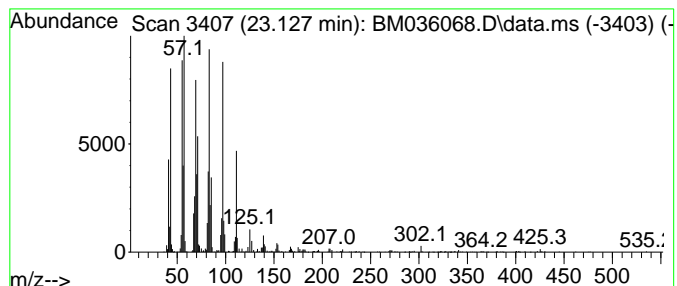
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 Peak Number 5 n-Tetracosanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.127	9.36 ng	1888430	Perylene-d12	23.785

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2		9-Tricosanol, acetate	382	C25H50O2	039754-92-2	91
3		Heptacos-1-ene	378	C27H54	015306-27-1	91
4		Octacosanol	410	C28H58O	000557-61-9	91
5		Pentacos-1-ene	350	C25H50	016980-85-1	91



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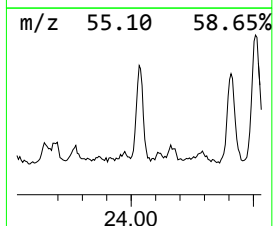
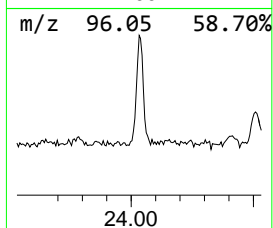
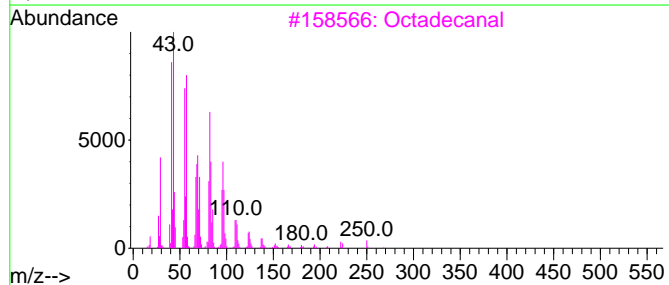
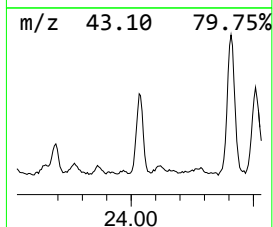
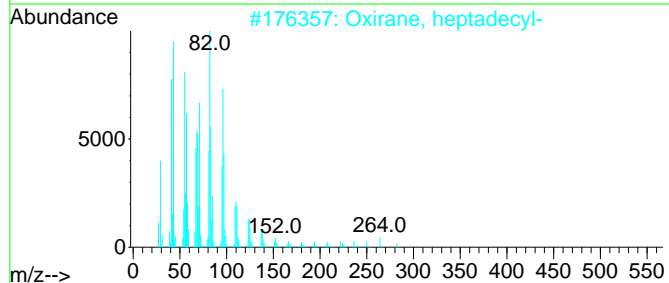
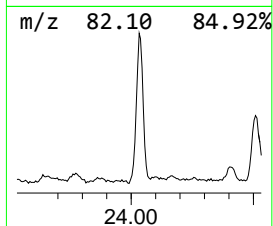
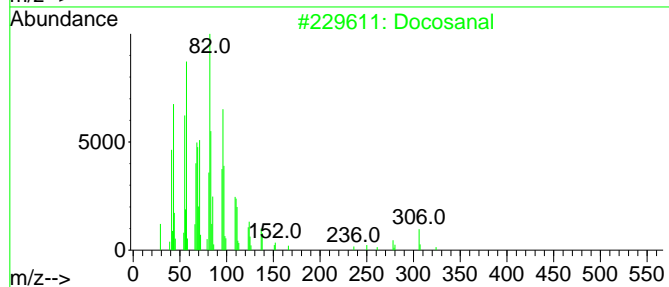
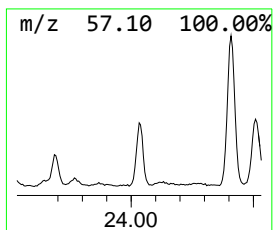
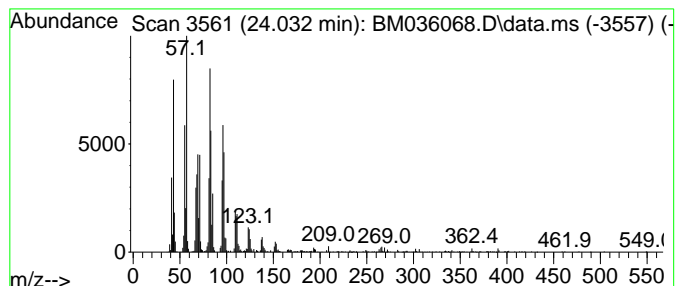
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 6 Docosanal Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.032	6.46 ng	1302890	Perylene-d12	23.785

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Docosanal	324	C22H44O	057402-36-5	93
2		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
3		Octadecanal	268	C18H36O	000638-66-4	90
4		Octacosanal	408	C28H56O	022725-64-0	90
5		Tetracosanal	352	C24H48O	057866-08-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080222\
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 Acq On : 03 Aug 2022 01:09
 Operator : CG/JU
 Sample : N3896-11
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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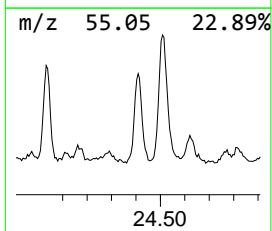
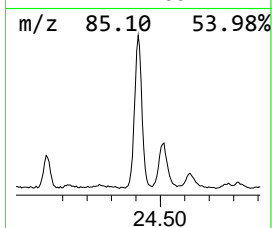
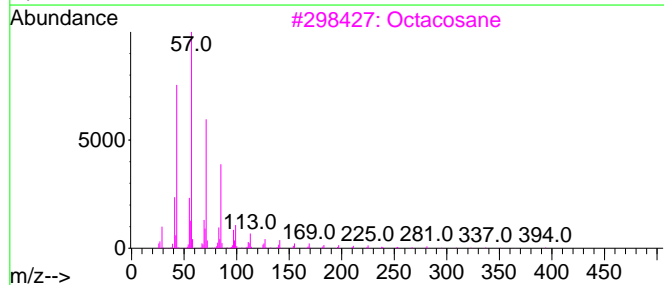
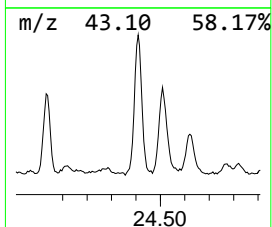
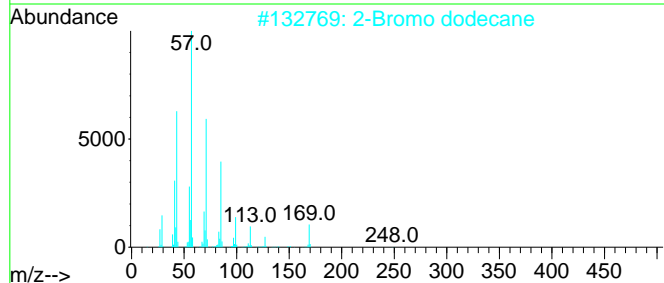
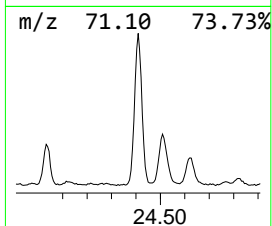
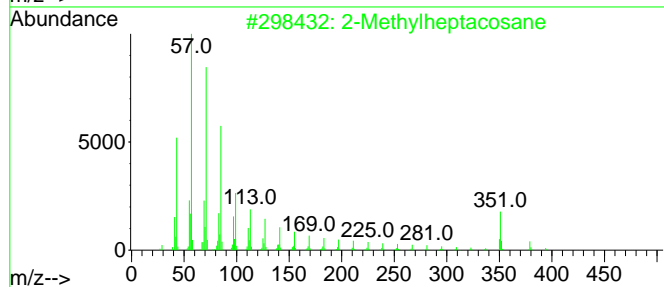
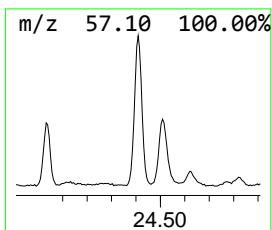
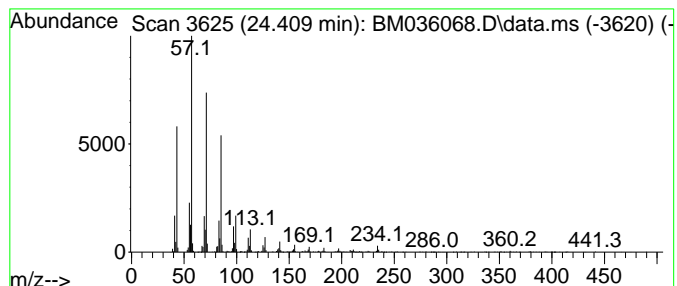
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 7 2-Methylheptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.409	8.56 ng	1726940	Perylene-d12	23.785

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Methylheptacosane	394	C28H58	001561-00-8	95
2		2-Bromo dodecane	248	C12H25Br	013187-99-0	93
3		Octacosane	394	C28H58	000630-02-4	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080222\
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Instrument :
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 ClientSampleId :
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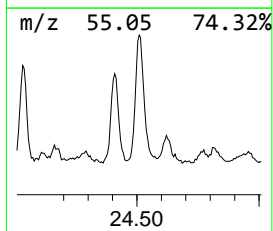
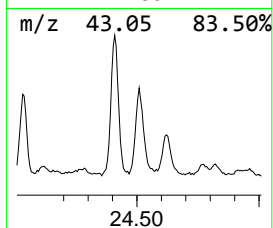
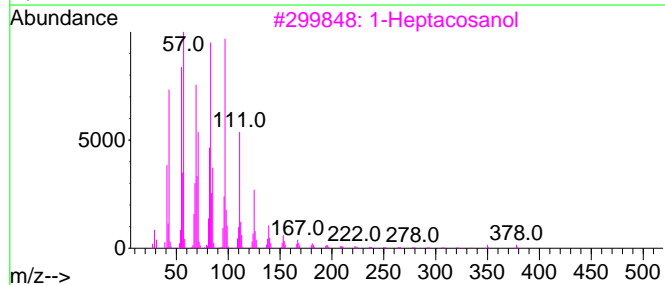
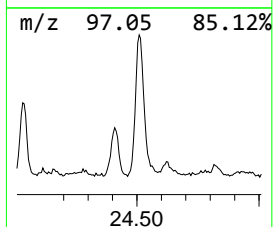
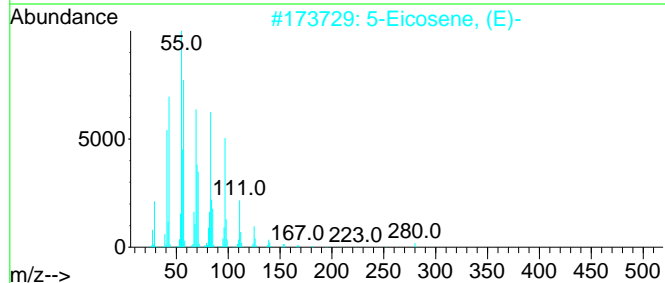
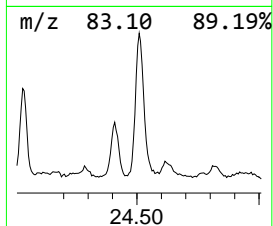
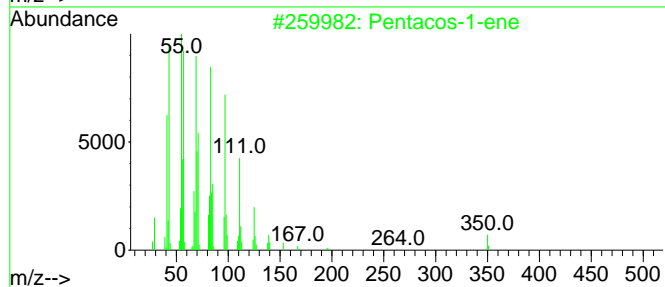
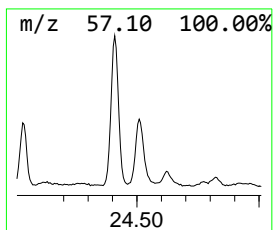
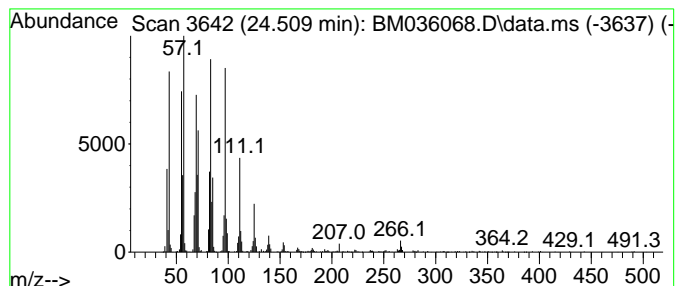
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 8 Pentacos-1-ene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.509	7.85 ng	1583020	Perylene-d12	23.785

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentacos-1-ene	350	C25H50	016980-85-1	96
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	95
3		1-Heptacosanol	396	C27H56O	002004-39-9	94
4		Heptacos-1-ene	378	C27H54	015306-27-1	94
5		1-Hexacosene	364	C26H52	018835-33-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080222\
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 Sample : N3896-11
 Misc :
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Instrument :
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 ClientSampleId :
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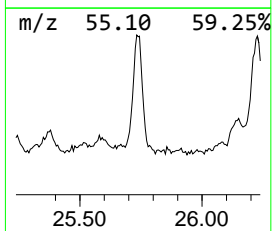
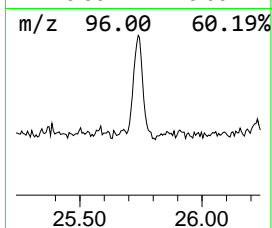
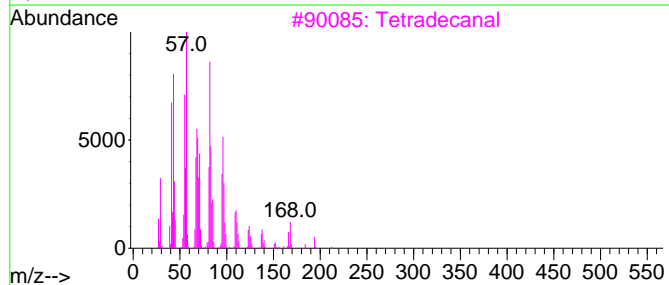
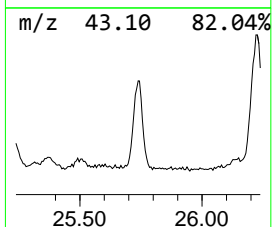
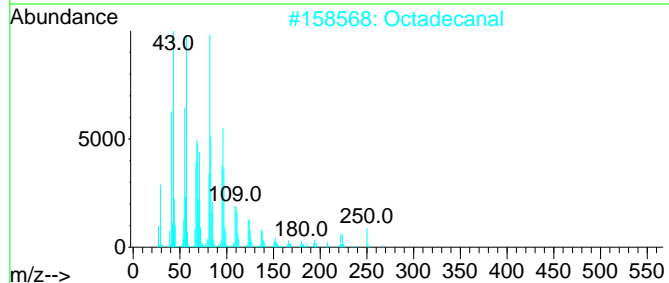
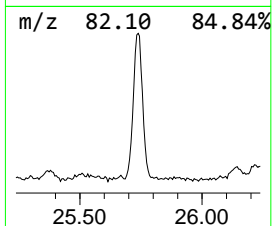
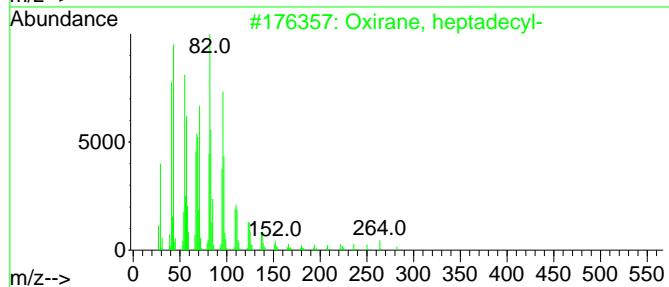
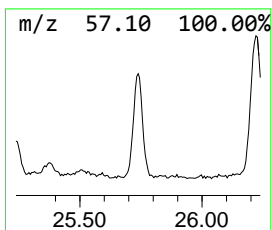
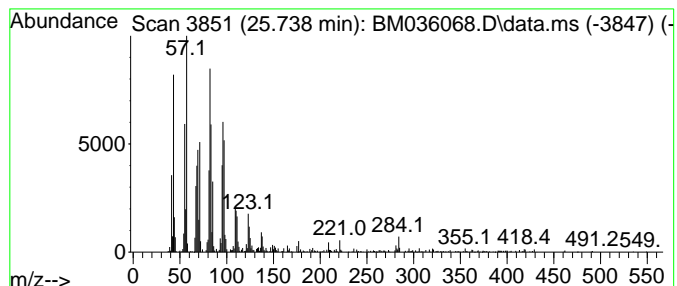
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 9 Oxirane, heptadecyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.738	7.25 ng	1462730	Perylene-d12	23.785

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
2		Octadecanal	268	C18H36O	000638-66-4	93
3		Tetradecanal	212	C14H28O	000124-25-4	91
4		Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	89
5		Nonacosanal	422	C29H58O	072934-04-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080222\
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 Sample : N3896-11
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Instrument :
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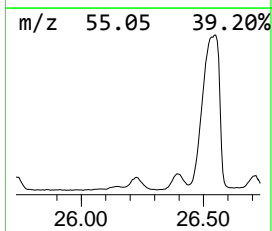
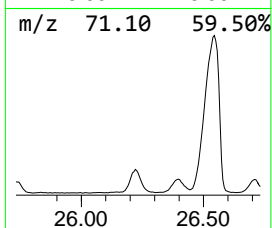
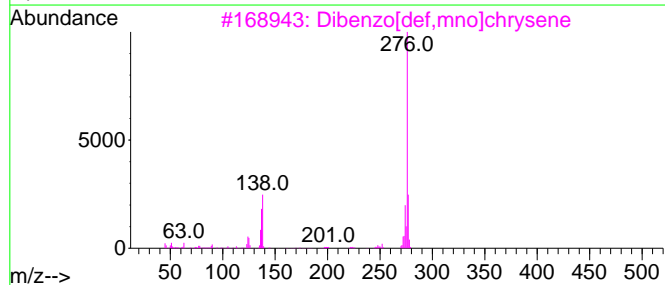
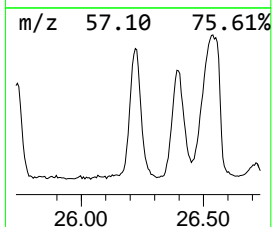
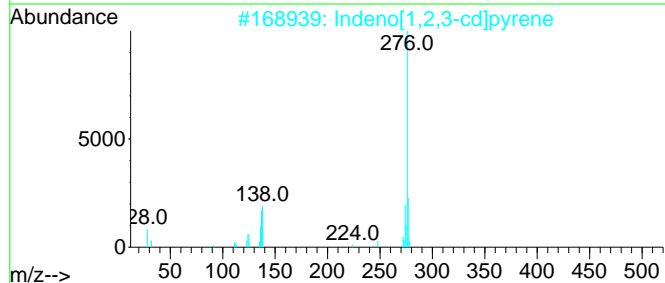
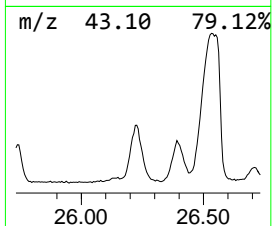
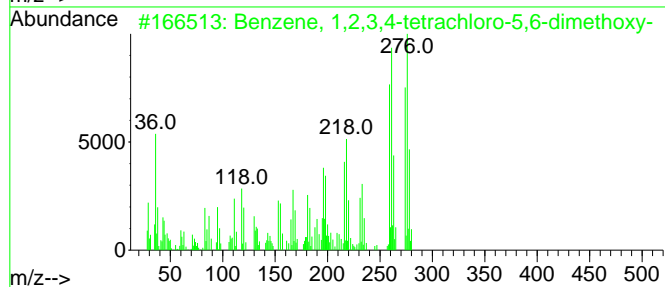
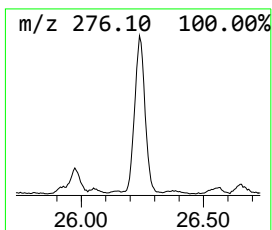
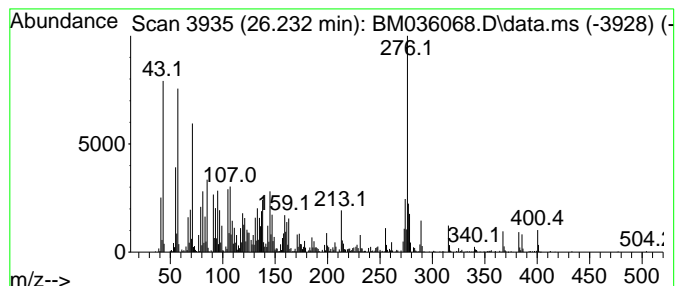
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 10 Benzene, 1,2,3,4-tetrachlor... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.232	17.14 ng	3456880	Perylene-d12	23.785

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,2,3,4-tetrachloro-5,6...	274	C8H6Cl4O2	000944-61-6	90
2		Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	90
3		Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	78
4		Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	60
5		Benzo[ghi]perylene	276	C22H12	000191-24-2	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080222\
 Data File : BM036068.D
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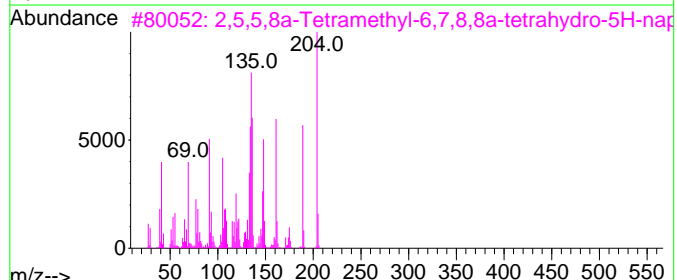
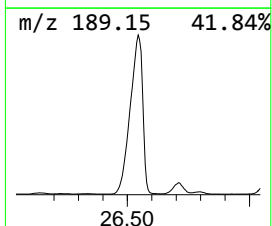
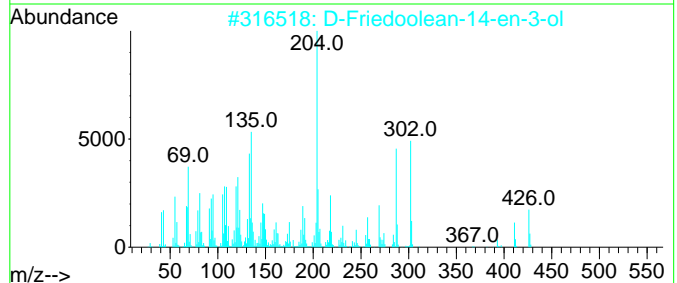
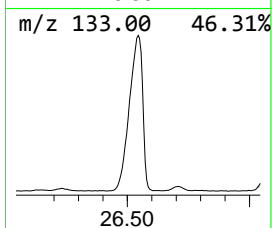
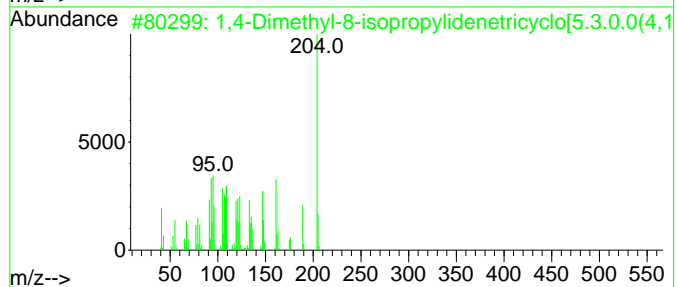
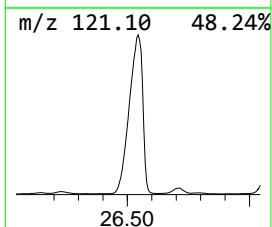
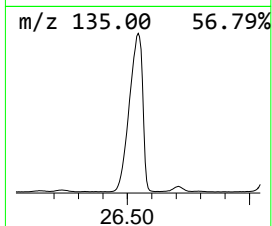
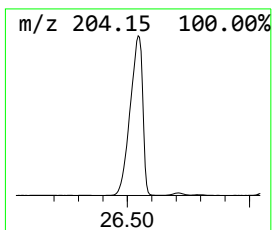
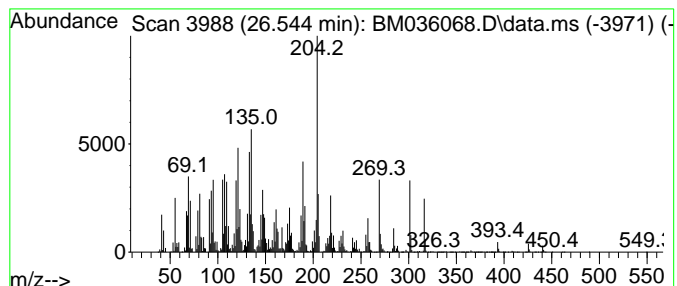
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 11 1,4-Dimethyl-8-isopropylide... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.544	492.38 ng	99289800	Perylene-d12	23.785

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	62
2		D-Friedoolean-14-en-3-ol	426	C30H50O	081654-73-1	62
3		2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	53
4		5-(2,4-Dichloro-phenoxyethyl)-4...	365	C16H13Cl2N3OS	1000296-81-4	46
5		1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080222\
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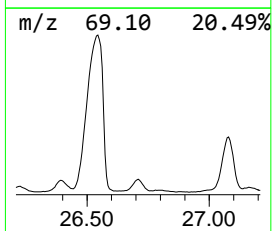
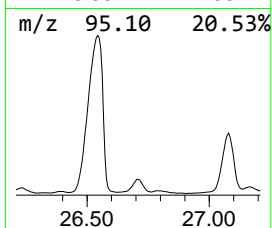
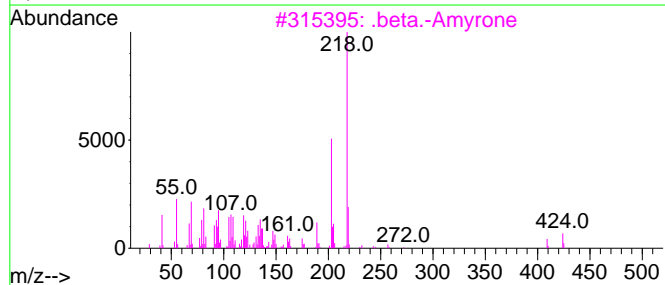
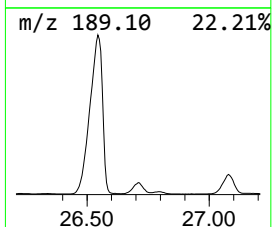
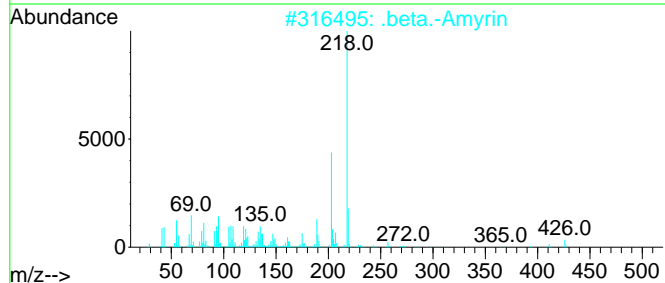
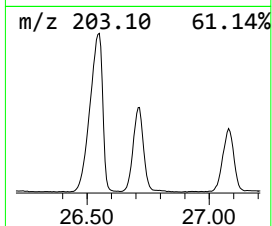
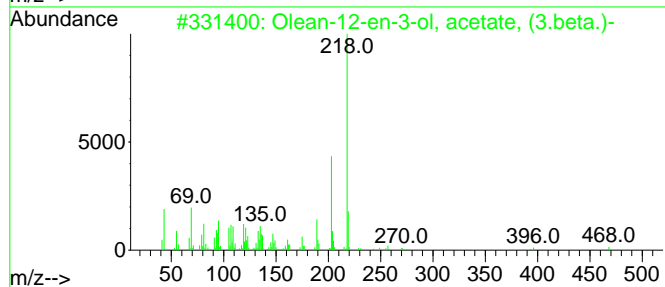
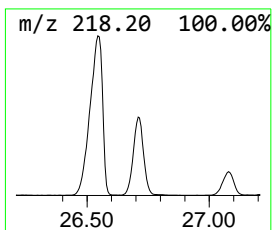
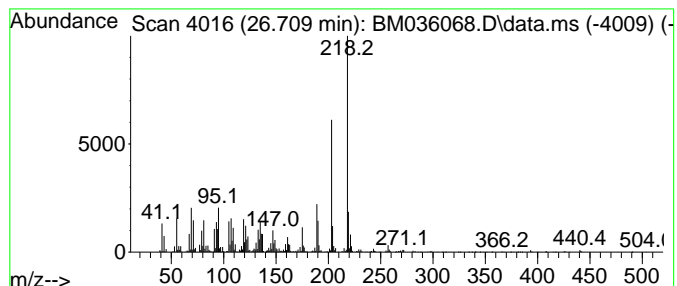
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 12 Olean-12-en-3-ol, acetate, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.709	18.91 ng	3812680	Perylene-d12	23.785

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Olean-12-en-3-ol, acetate, (3.be...	468	C32H52O2	001616-93-9	90
2		.beta.-Amyrin	426	C30H50O	000559-70-6	86
3		.beta.-Amyrone	424	C30H48O	000638-97-1	83
4		24-Noroleana-3,12-diene	394	C29H46	201358-24-9	83
5		.alpha.-Boswellic acid, 0,0-bis-...	484	C32H52O3	1010507-05-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080222\
 Data File : BM036068.D
 Acq On : 03 Aug 2022 01:09
 Operator : CG/JU
 Sample : N3896-11
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RVE-68

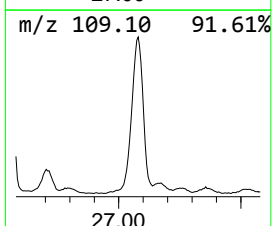
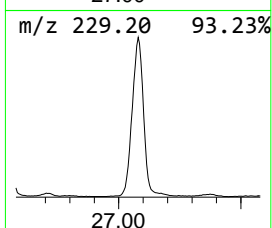
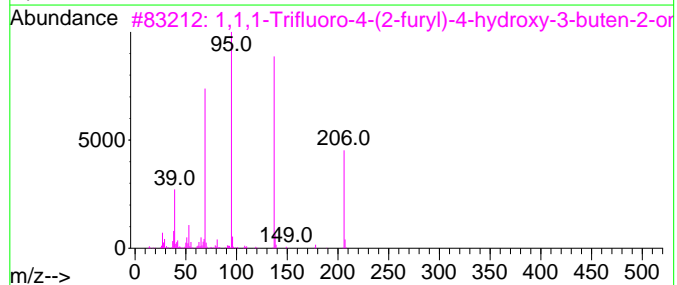
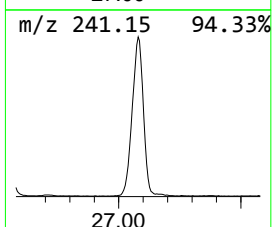
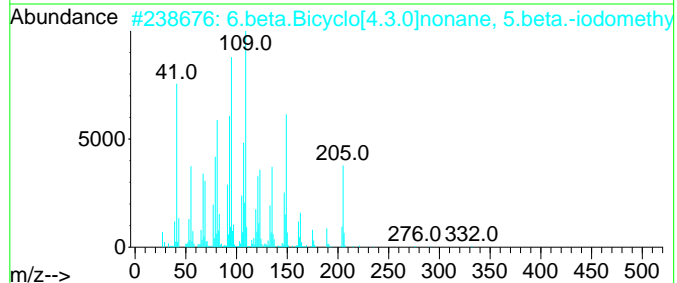
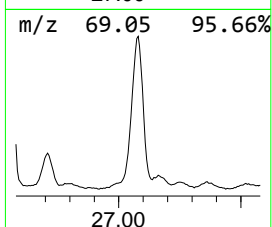
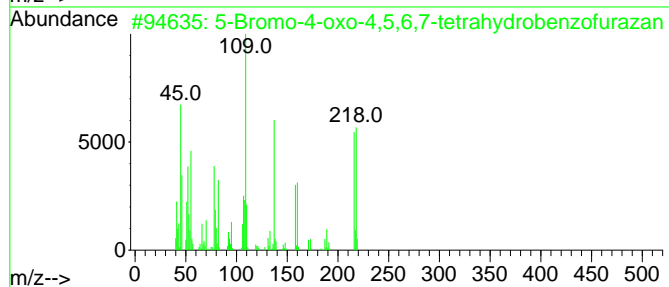
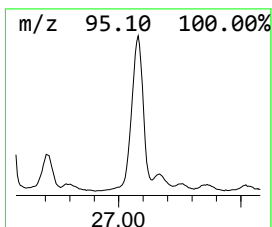
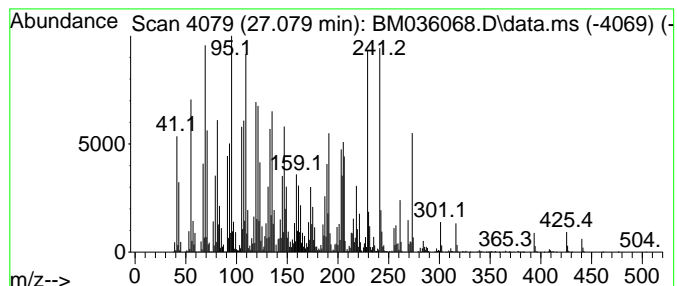
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 13 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.079	83.06 ng	16749400	Perylene-d12	23.785

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	90
2		6.beta.Bicyclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	27
3		1,1,1-Trifluoro-4-(2-furyl)-4-hy...	206	C8H5F3O3	015788-03-1	25
4		Furan-2-carboxamide, N-ethyl-N-(...	229	C14H15N2O2	1000308-20-3	20
5		2-(4-Fluorobenzyl)-2-azaspiro[4...	261	C15H16FN2	1000332-10-7	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080222\
 Data File : BM036068.D
 Acq On : 03 Aug 2022 01:09
 Operator : CG/JU
 Sample : N3896-11
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RVE-68

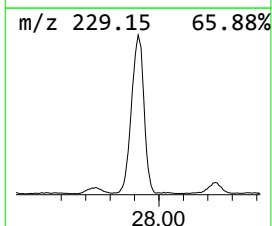
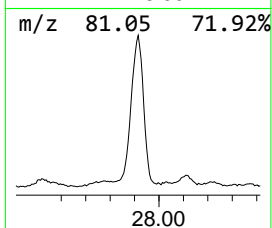
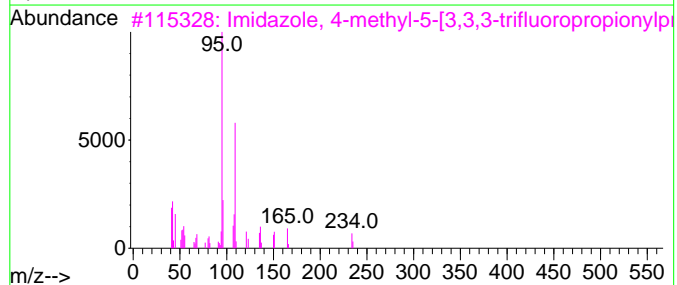
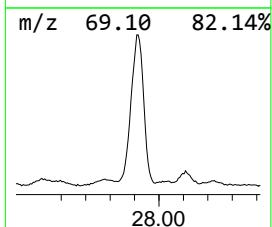
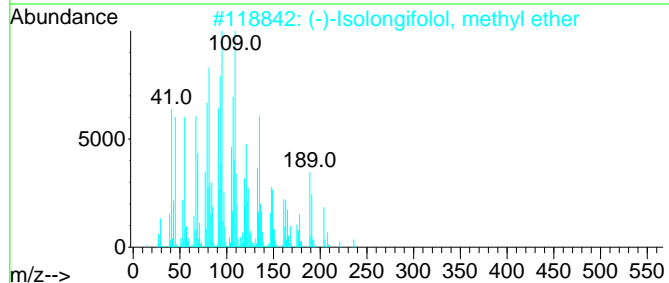
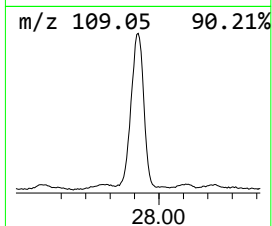
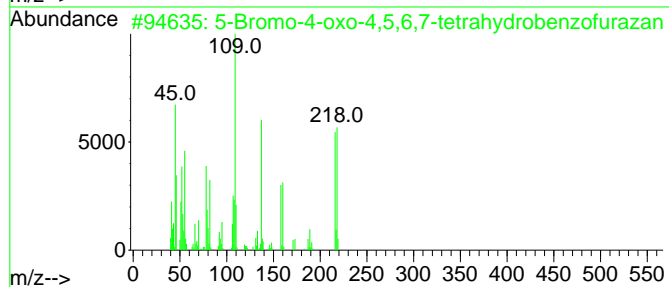
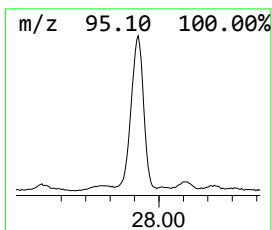
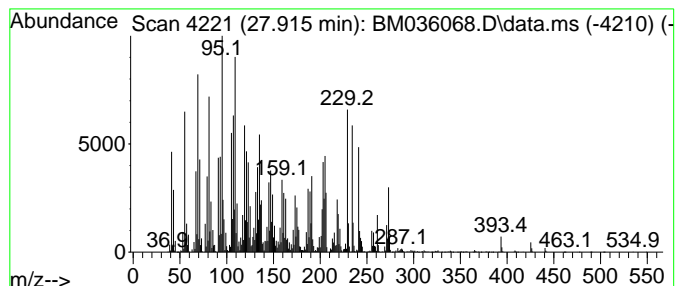
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 14 unknown27.915 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.915	81.84 ng	16503400	Perylene-d12	23.785

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	90
2		(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	46
3		Imidazole, 4-methyl-5-[3,3,3-tri...	234	C10H13F3N2O	1000129-15-8	41
4		9-Thiabicyclo[3.3.1]nonane, 2,6-...	274	C14H18N4S	1000141-52-1	35
5		5-Methoxy-10,10-dimethyl-6-methy...	236	C15H24O2	1000511-71-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080222\
 Data File : BM036068.D
 Acq On : 03 Aug 2022 01:09
 Operator : CG/JU
 Sample : N3896-11
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RVE-68

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.151	12.5	ng	2826230	4	17.245	4532980	20.0
Ethanol, 2-(tet...	21.139	12.9	ng	3905500	5	21.421	6076550	20.0
1-Docosanol, me...	22.056	3.5	ng	1065240	5	21.421	6076550	20.0
Hexacosanal	22.774	9.6	ng	1932720	6	23.785	4033050	20.0
n-Tetracosanol-1	23.127	9.4	ng	1888430	6	23.785	4033050	20.0
Docosanal	24.032	6.5	ng	1302890	6	23.785	4033050	20.0
2-Methylheptaco...	24.409	8.6	ng	1726940	6	23.785	4033050	20.0
Pentacos-1-ene	24.509	7.8	ng	1583020	6	23.785	4033050	20.0
Oxirane, heptad...	25.738	7.3	ng	1462730	6	23.785	4033050	20.0
Benzene, 1,2,3,...	26.232	17.1	ng	3456880	6	23.785	4033050	20.0
1,4-Dimethyl-8-...	26.544	492.4	ng	99289800	6	23.785	4033050	20.0
Olean-12-en-3-o...	26.709	18.9	ng	3812680	6	23.785	4033050	20.0
5-Bromo-4-oxo-4...	27.079	83.1	ng	16749400	6	23.785	4033050	20.0
unknown27.915	27.915	81.8	ng	16503400	6	23.785	4033050	20.0