

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092821\
 Data File : BF125689.D
 Acq On : 28 Sep 2021 15:20
 Operator : JU/CG
 Sample : M3953-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-RR-03-(SA)

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_F\METHODS\8270-BF092421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125689.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	8	15	21	rBV	4350160	5991602	89.68%	13.602%
2	5.498	576	580	584	rBV	3122594	2995401	44.83%	6.800%
3	6.498	746	750	756	rBV	2216324	1930449	28.89%	4.383%
4	6.886	812	816	819	rBV	1530397	1169265	17.50%	2.654%
5	7.445	906	911	914	rBV	3839281	3630091	54.33%	8.241%
6	8.063	1013	1016	1030	rBV	198406	205261	3.07%	0.466%
7	8.169	1030	1034	1037	rBV	1953499	1632155	24.43%	3.705%
8	9.245	1212	1217	1220	rBV	7478428	6681458	100.00%	15.168%
9	9.921	1328	1332	1335	rBV	2304676	1784045	26.70%	4.050%
10	10.327	1397	1401	1407	rVB	186280	218685	3.27%	0.496%
11	10.710	1461	1466	1469	rBV	4354059	3919330	58.66%	8.898%
12	10.798	1476	1481	1490	rBV2	163335	198447	2.97%	0.451%
13	11.404	1580	1584	1588	rBV	1993034	1706410	25.54%	3.874%
14	11.927	1667	1673	1688	rBV2	564953	710713	10.64%	1.613%
15	12.715	1802	1807	1817	rBV	211544	275481	4.12%	0.625%
16	12.992	1849	1854	1857	rBV	6367709	5957167	89.16%	13.524%
17	13.262	1884	1900	1910	rBV4	62116	299135	4.48%	0.679%
18	13.892	2001	2007	2008	rBV2	148940	182814	2.74%	0.415%
19	14.039	2025	2032	2053	rBV	1468098	1771962	26.52%	4.023%
20	14.439	2094	2100	2110	rBV3	104227	304637	4.56%	0.692%
21	14.698	2137	2144	2154	rVB10	40903	130524	1.95%	0.296%
22	14.862	2167	2172	2184	rVB3	96889	237396	3.55%	0.539%
23	15.345	2246	2254	2268	rVB4	74411	258910	3.88%	0.588%
24	15.515	2277	2283	2288	rBV	869161	1106886	16.57%	2.513%
25	16.409	2428	2435	2450	rVB3	46111	152459	2.28%	0.346%
26	17.386	2592	2601	2618	rVB5	151797	598165	8.95%	1.358%

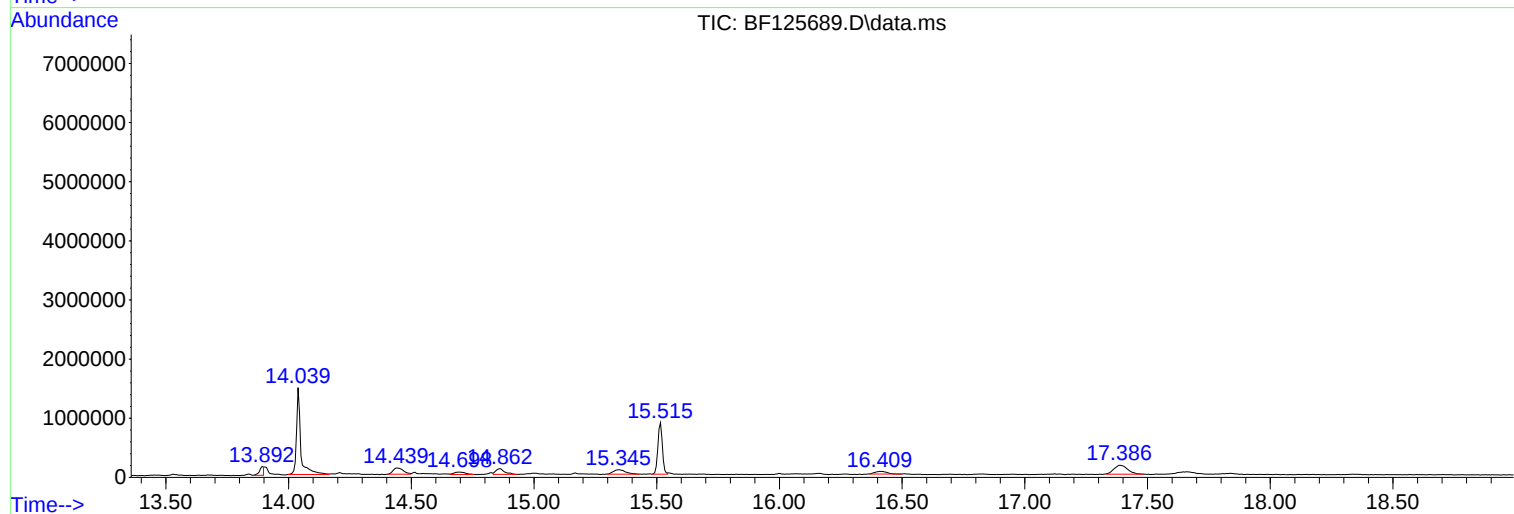
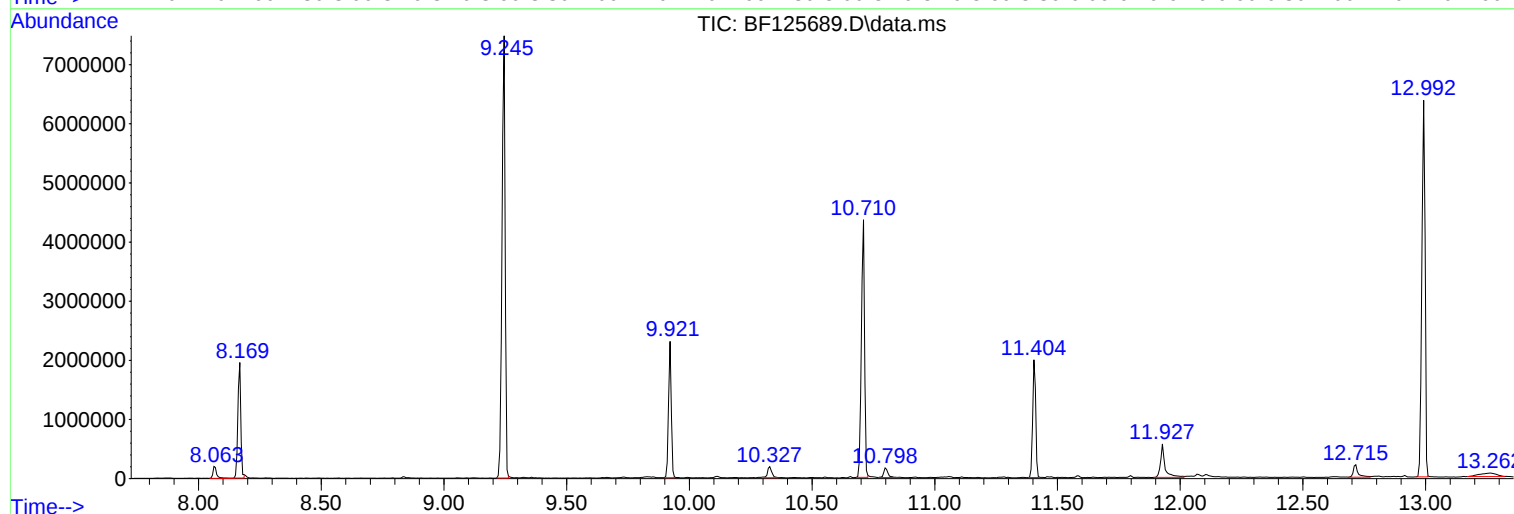
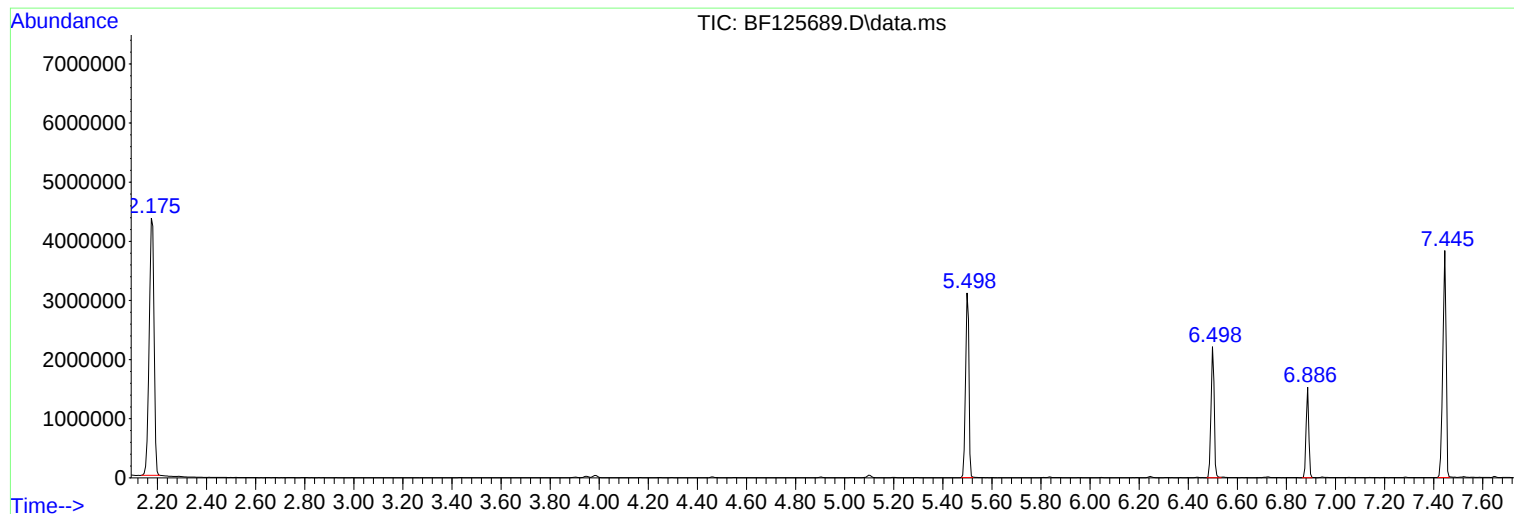
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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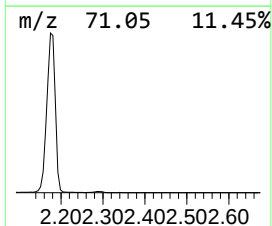
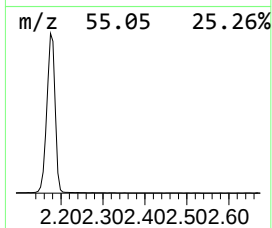
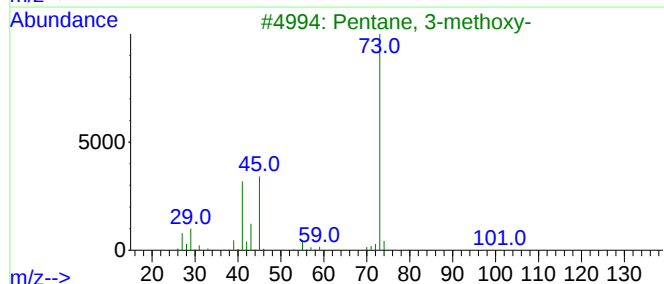
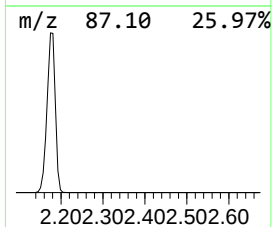
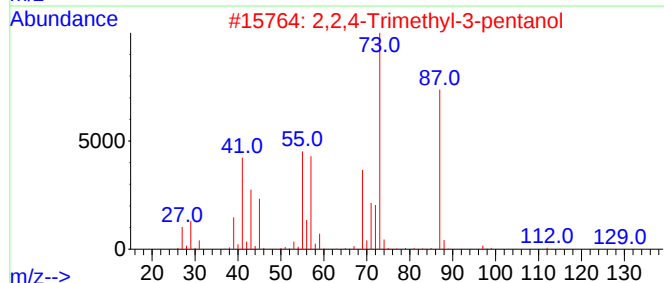
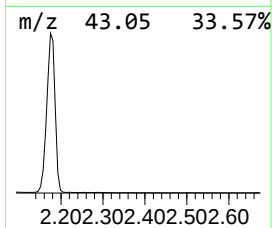
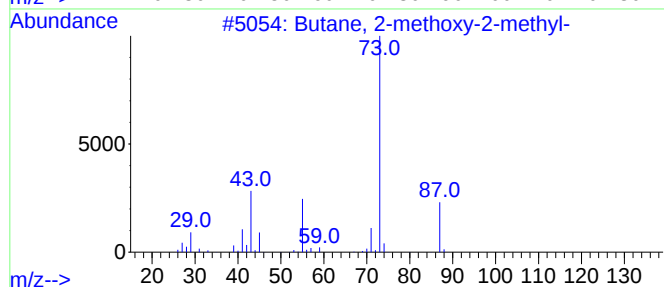
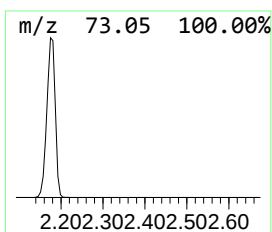
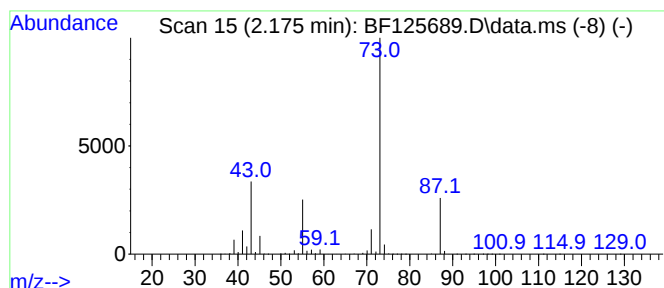
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	102.49 ng	5991600	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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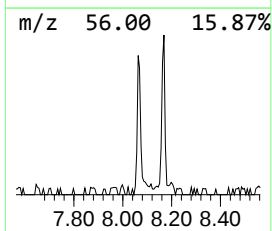
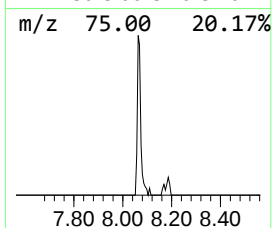
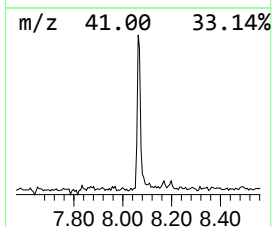
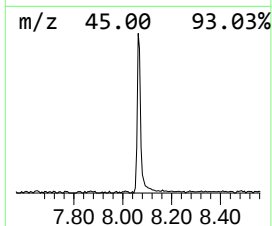
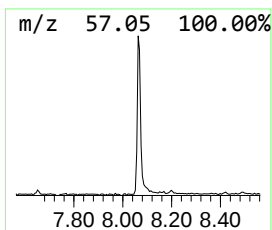
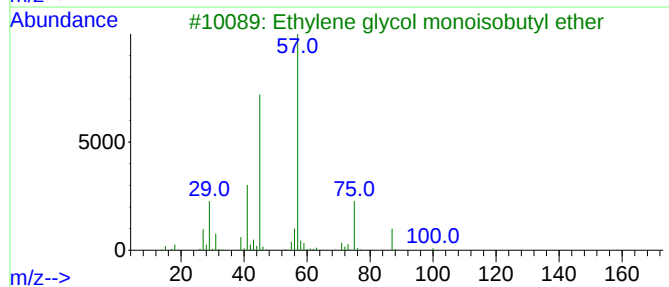
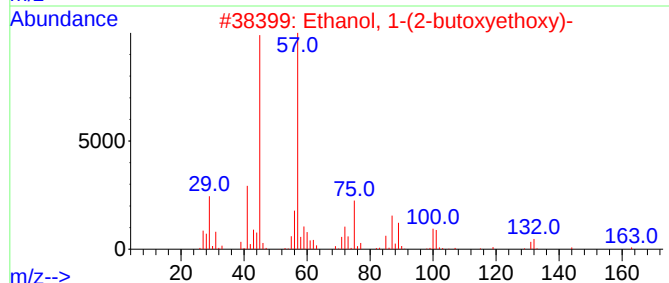
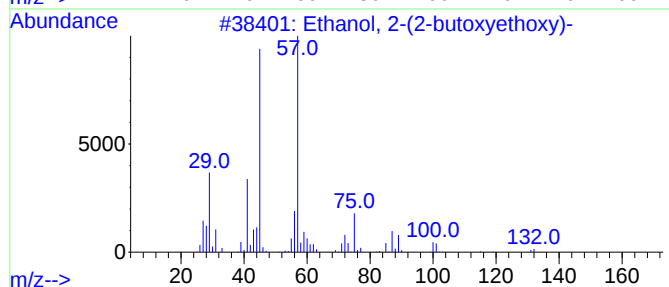
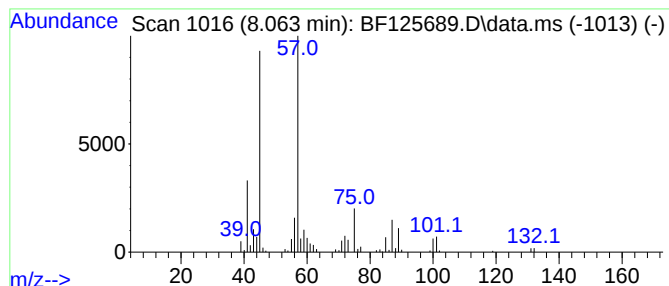
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.063	2.52 ng	205261	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53



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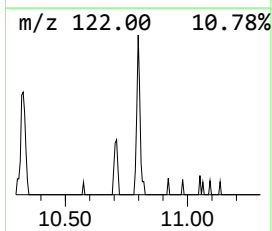
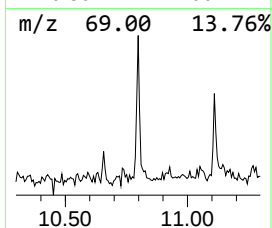
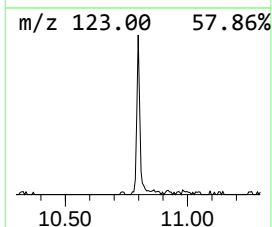
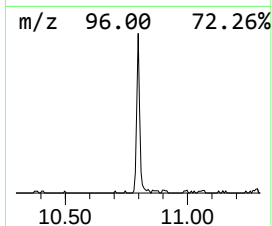
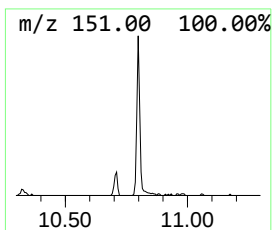
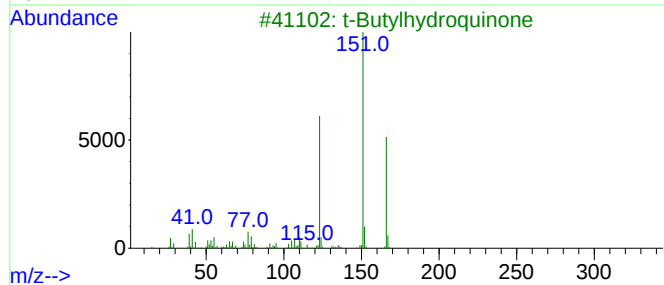
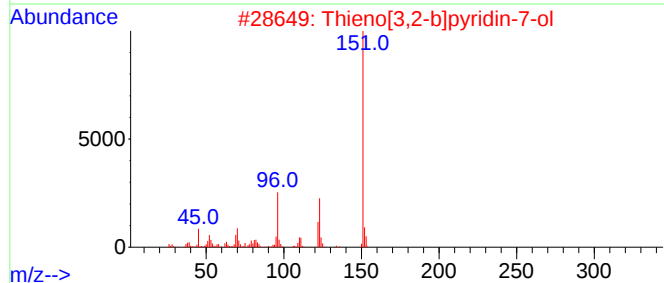
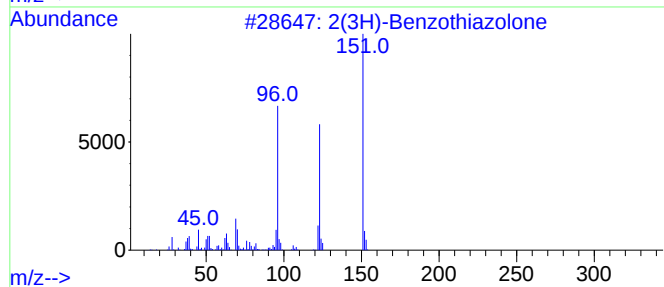
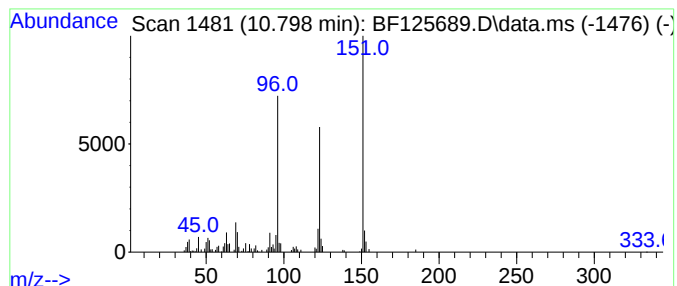
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2(3H)-Benzothiazolone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.798	2.33 ng	198447	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	96
2			Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	64
3			t-Butylhydroquinone	166	C10H14O2	001948-33-0	50
4			1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	49
5			4-Methoxyformanilide	151	C8H9NO2	005470-34-8	43



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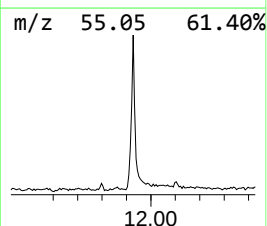
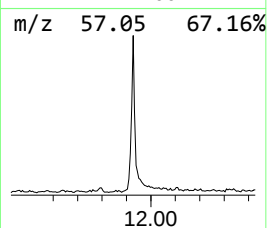
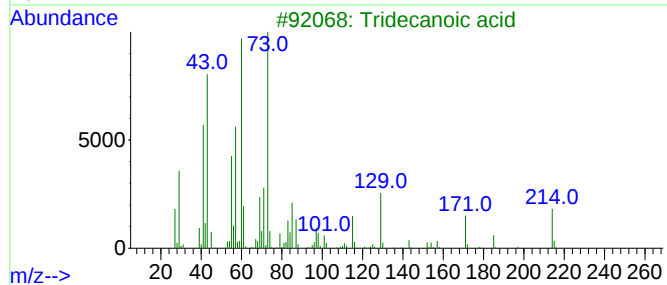
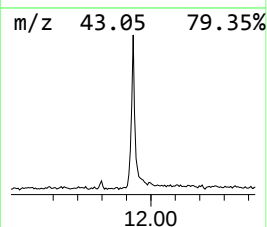
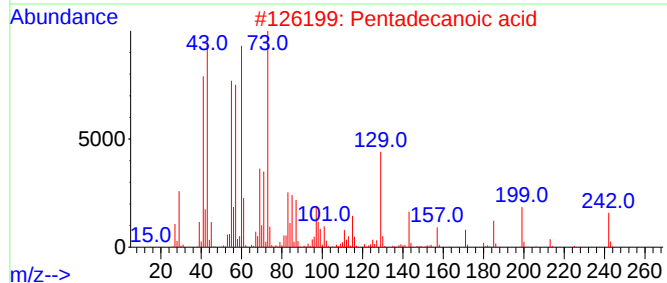
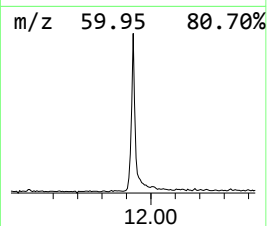
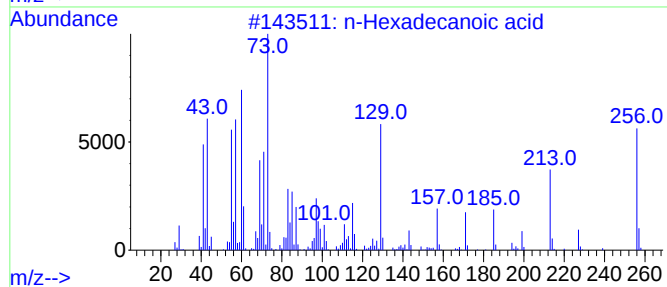
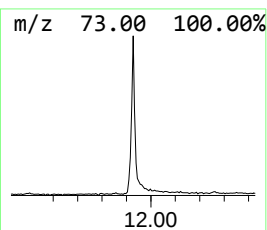
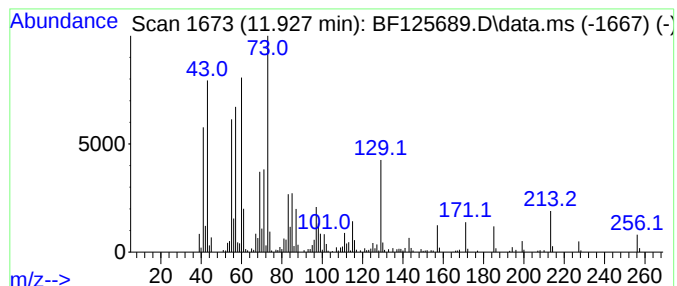
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	8.33 ng	710713	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5			Undecanoic acid	186	C11H22O2	000112-37-8	86



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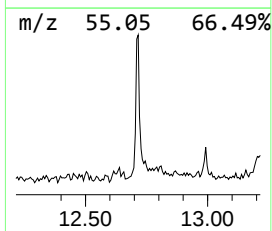
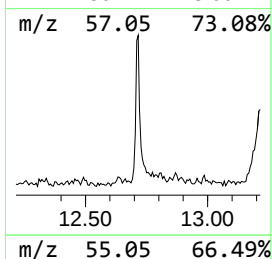
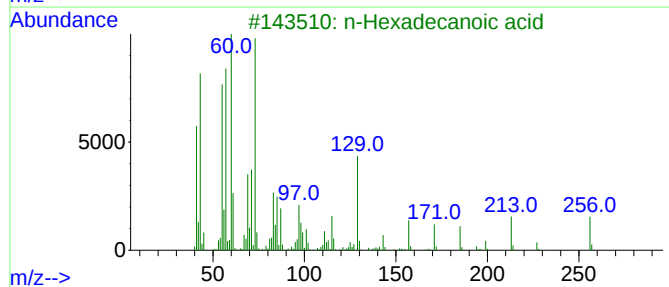
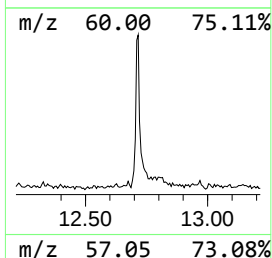
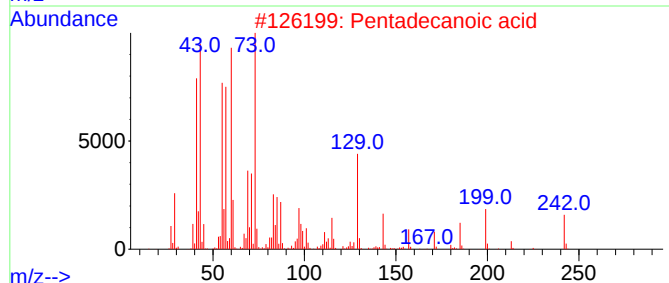
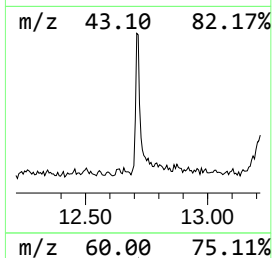
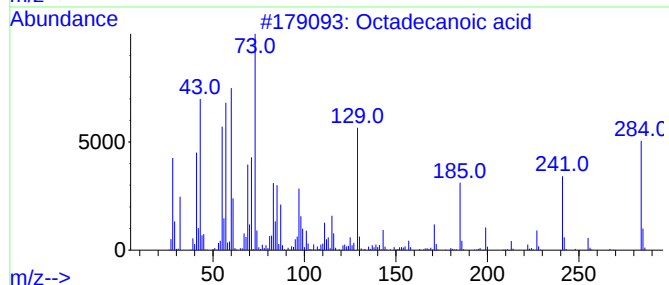
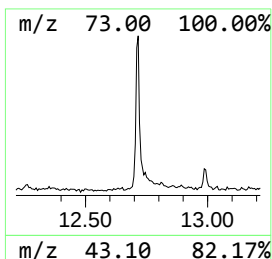
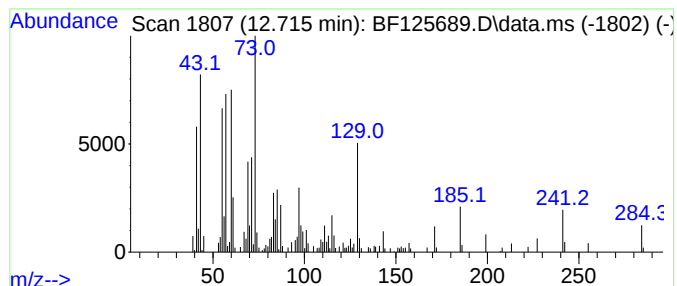
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Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.715	3.23 ng	275481	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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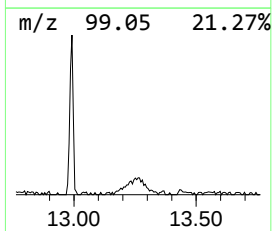
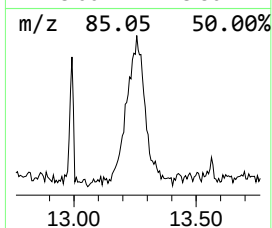
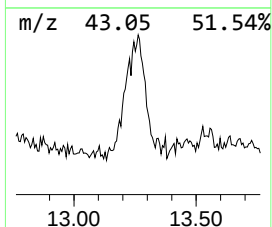
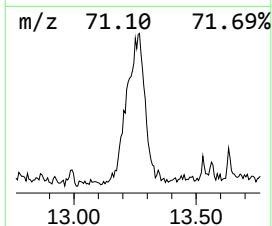
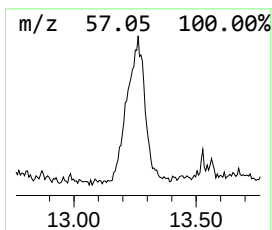
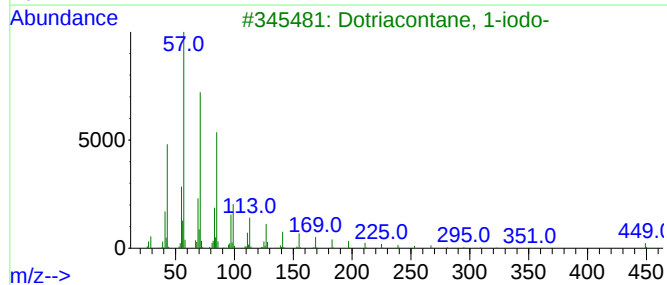
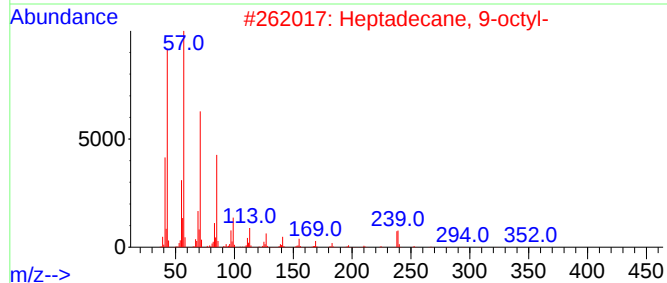
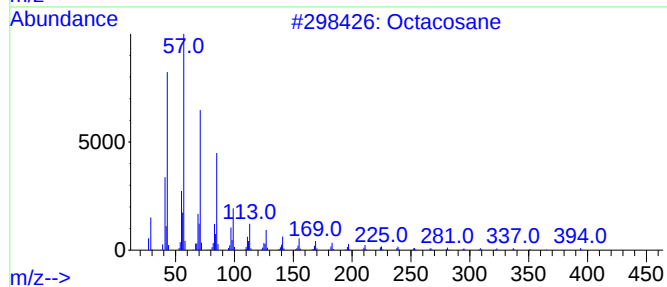
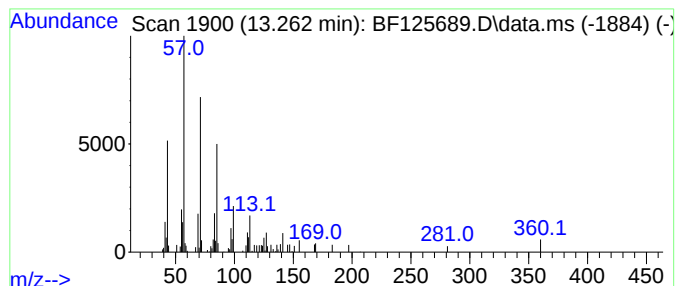
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.262	3.38 ng	299135	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Pentacosane	352	C25H52	000629-99-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092821\
Data File : BF125689.D
Acq On : 28 Sep 2021 15:20
Operator : JU/CG
Sample : M3953-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

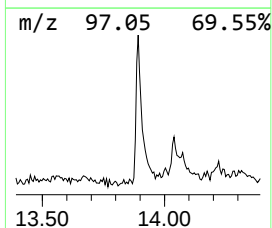
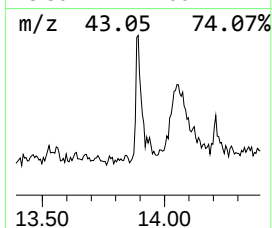
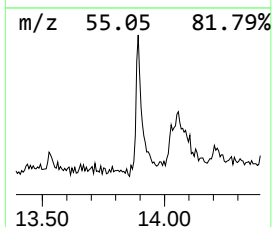
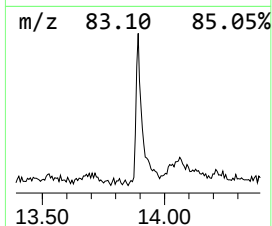
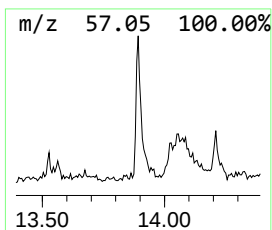
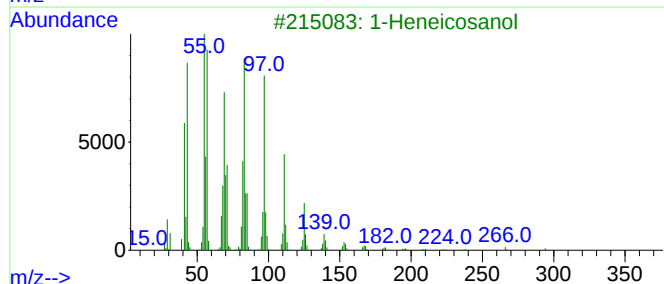
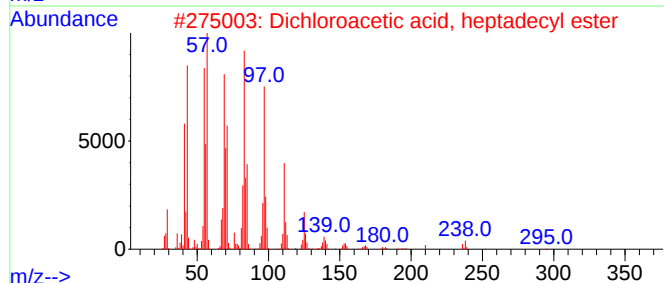
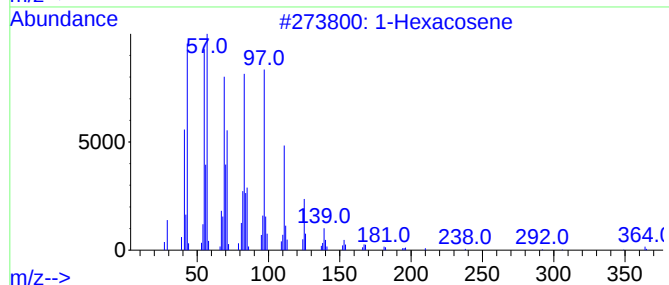
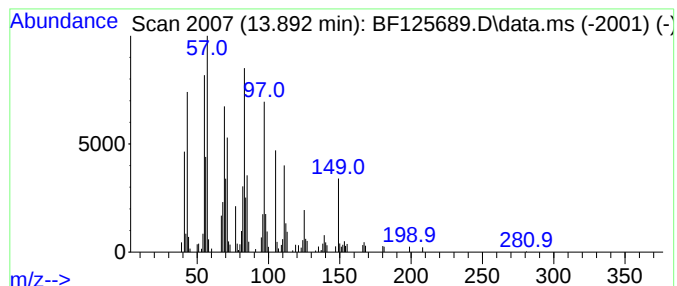
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ClientSampleId :
SW-RR-03-(SA)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Hexacosene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.892	2.06 ng	182814	Chrysene-d12	14.039	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	93
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092821\
Data File : BF125689.D
Acq On : 28 Sep 2021 15:20
Operator : JU/CG
Sample : M3953-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-RR-03-(SA)

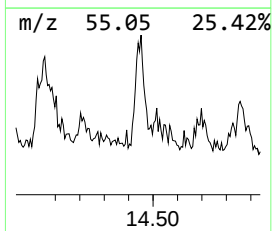
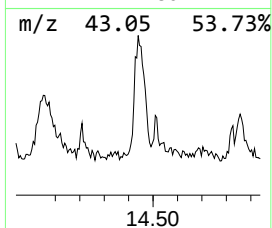
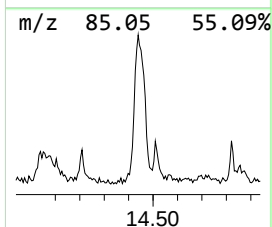
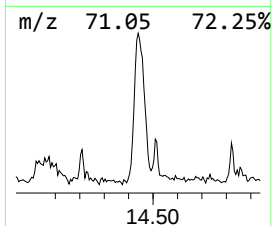
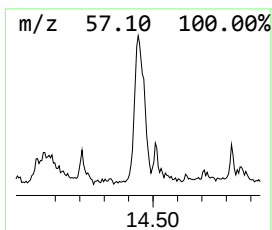
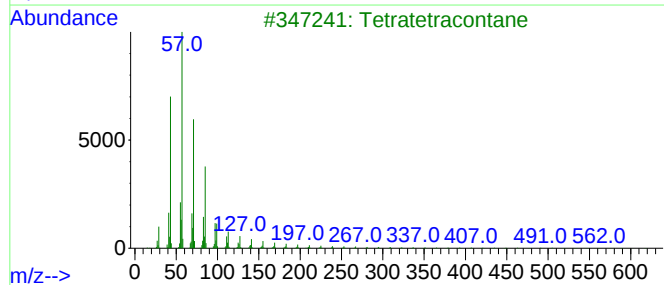
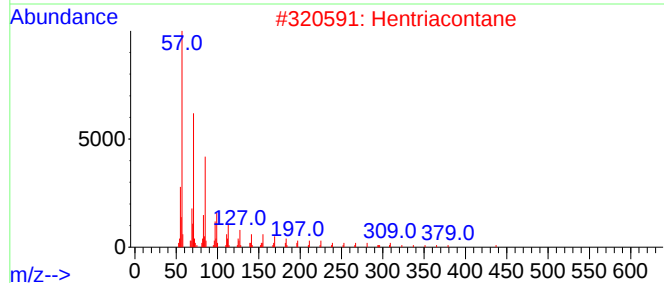
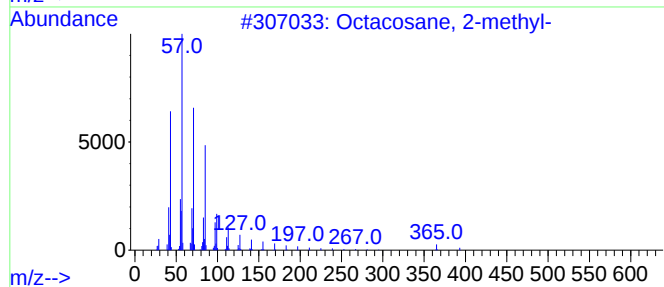
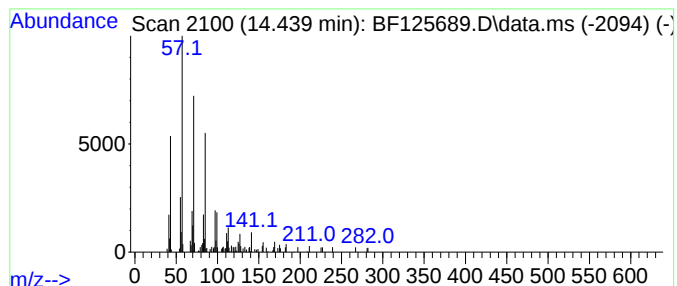
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.439	3.44 ng	304637	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Hentriacontane	437	C31H64	000630-04-6	90
3			Tetratetracontane	619	C44H90	007098-22-8	90
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092821\
Data File : BF125689.D
Acq On : 28 Sep 2021 15:20
Operator : JU/CG
Sample : M3953-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-RR-03-(SA)

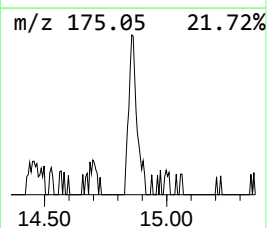
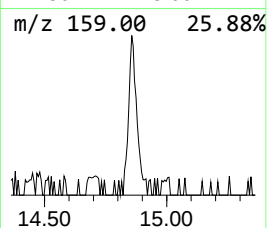
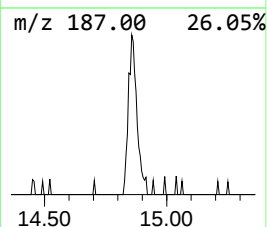
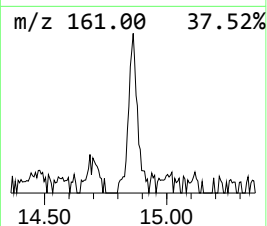
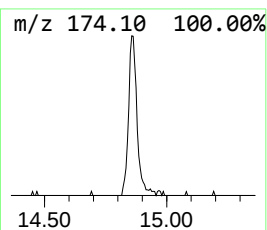
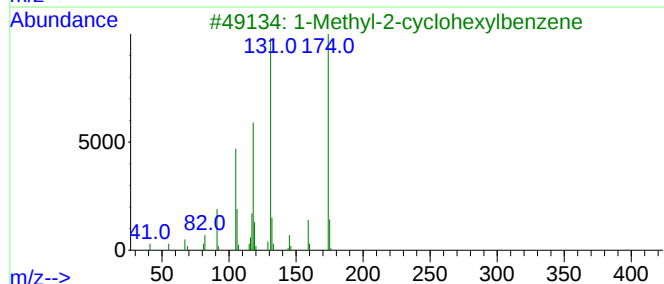
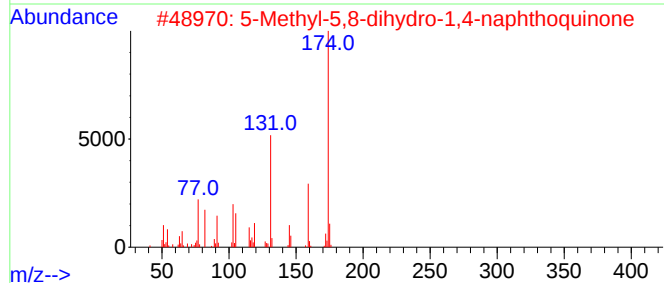
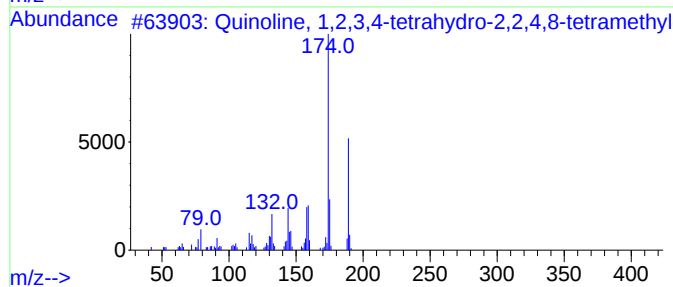
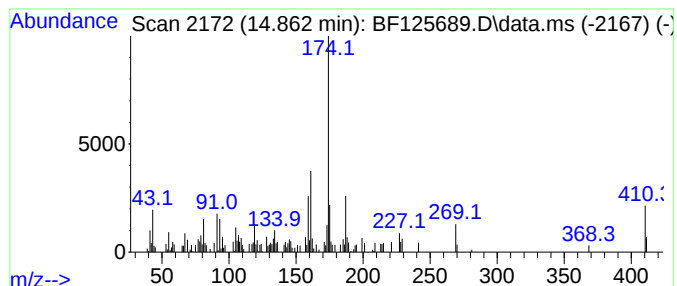
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.862 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.862	4.29 ng	237396	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Quinoline, 1,2,3,4-tetrahydro-2,...	189	C13H19N	1000308-78-8	47		
2	5-Methyl-5,8-dihydro-1,4-naphtho...	174	C11H10O2	086759-40-2	38		
3	1-Methyl-2-cyclohexylbenzene	174	C13H18	004501-35-3	38		
4	1-Ethyl-N-[4-(piperidin-1-yl)ben...	286	C15H22N6	1010482-38-1	38		
5	Quinazoline, 4-ethyl-, 3-oxide	174	C10H10N2O	037920-74-4	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092821\
Data File : BF125689.D
Acq On : 28 Sep 2021 15:20
Operator : JU/CG
Sample : M3953-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

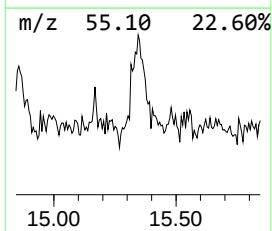
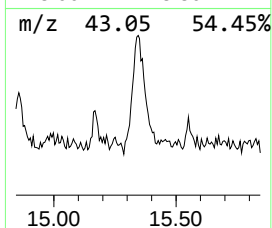
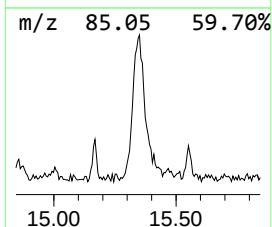
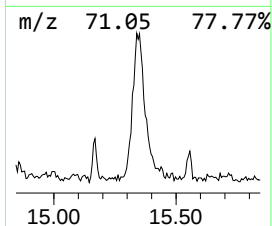
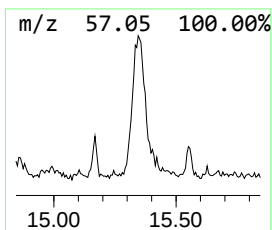
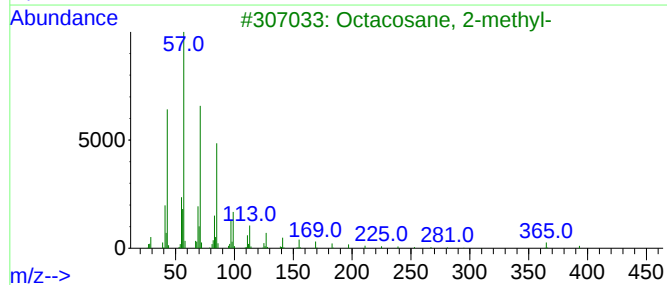
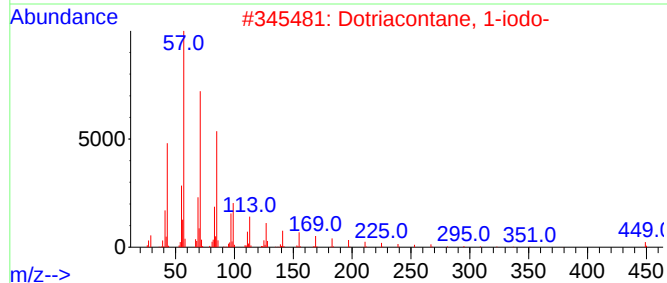
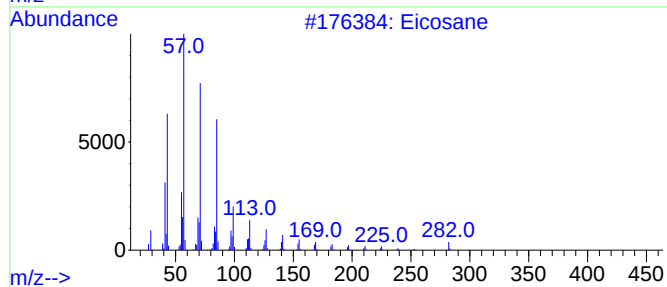
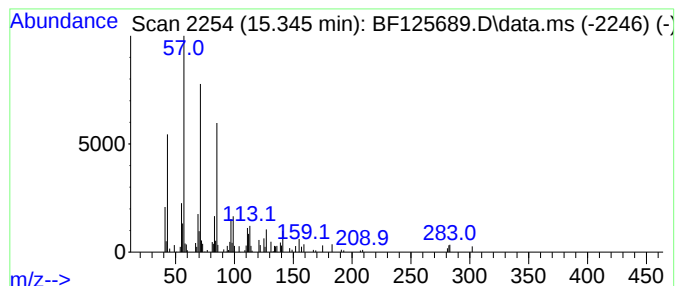
Instrument :
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ClientSampleId :
SW-RR-03-(SA)

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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 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.345	4.68 ng	258910	Perylene-d12	15.515	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092821\
Data File : BF125689.D
Acq On : 28 Sep 2021 15:20
Operator : JU/CG
Sample : M3953-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-RR-03-(SA)

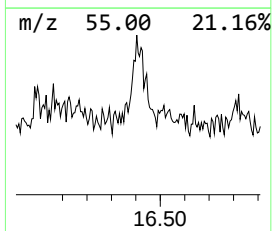
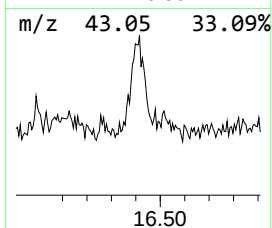
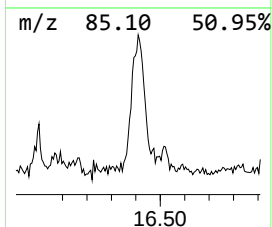
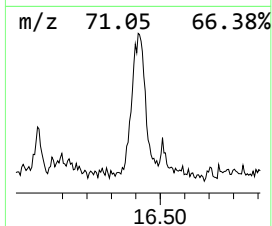
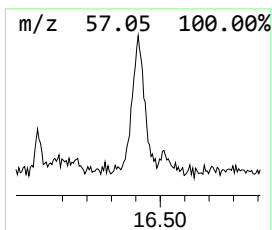
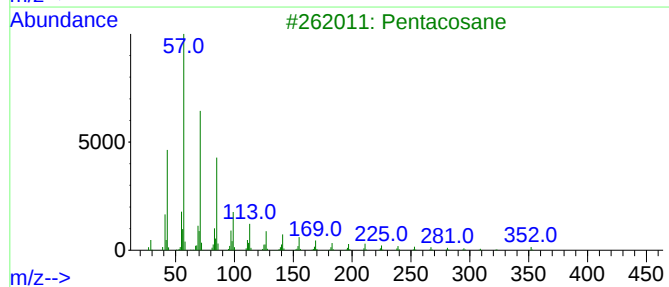
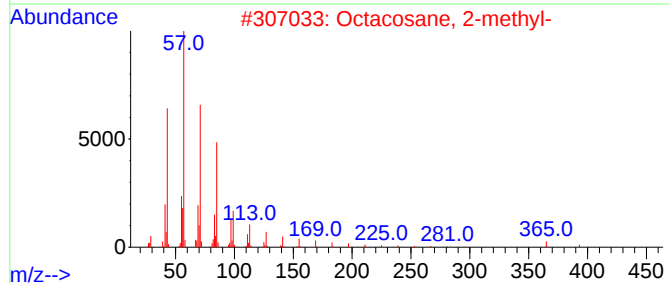
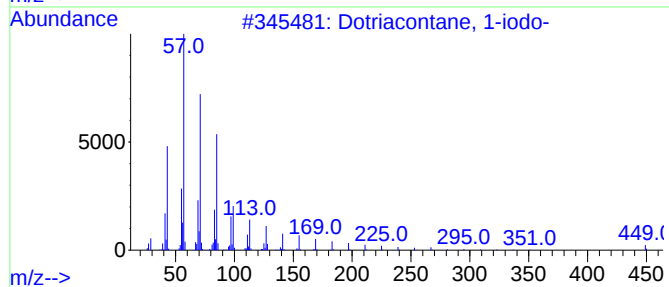
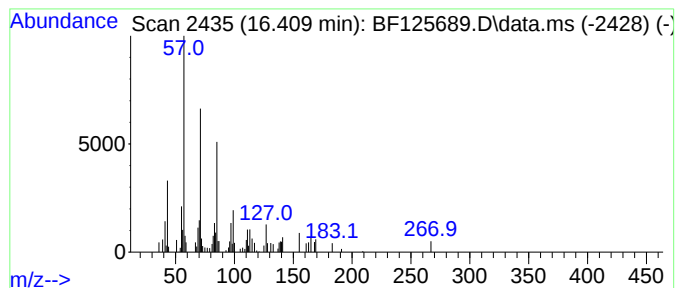
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Dotriacontane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.409	2.75 ng	152459	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Pentacosane	352	C25H52	000629-99-2	90
4			Heptacosane	380	C27H56	000593-49-7	90
5			Triacontane	422	C30H62	000638-68-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092821\
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Acq On : 28 Sep 2021 15:20
Operator : JU/CG
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-RR-03-(SA)

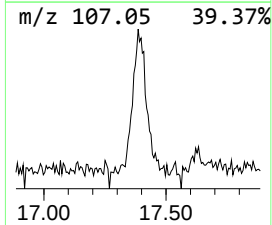
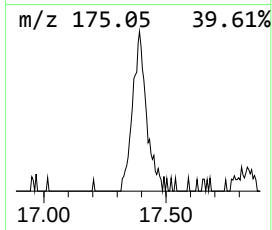
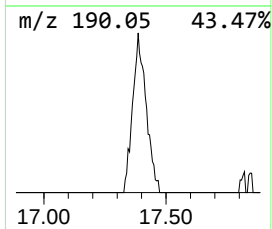
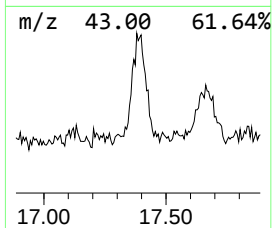
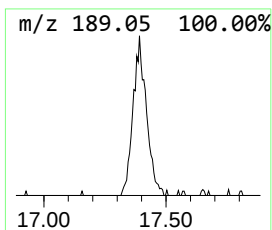
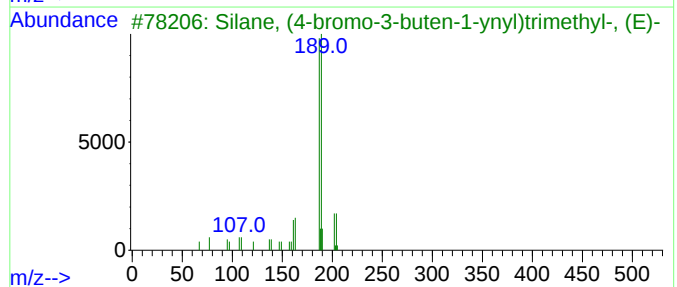
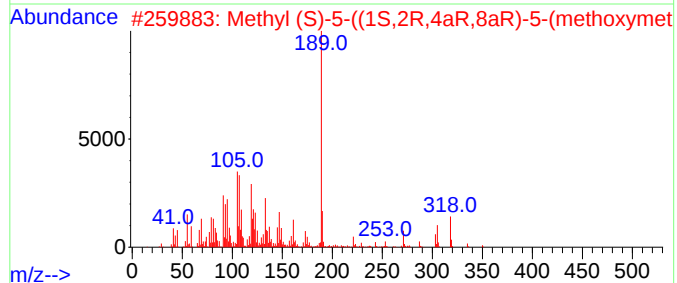
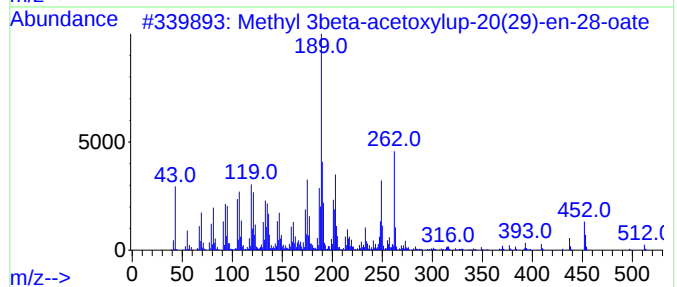
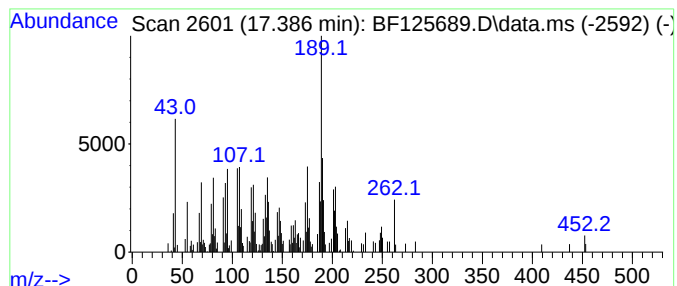
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Methyl 3beta-acetoxylup-20(... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.386	10.81 ng	598165	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 3beta-acetoxylup-20(29)-e...	512	C33H52O4	004356-30-3	90
2			Methyl (S)-5-((1S,2R,4aR,8aR)-5-...	350	C22H38O3	1010495-83-9	45
3			Silane, (4-bromo-3-buten-1-ynyl)...	202	C7H11BrSi	107646-62-8	43
4			2-(Hydroxymethyl)-2,4-dimethyl-4...	260	C15H16O4	1005254-37-4	38
5			2-Naphthalenemethanol, 1,2,3,4,4...	222	C15H26O	001209-71-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092821\
Data File : BF125689.D
Acq On : 28 Sep 2021 15:20
Operator : JU/CG
Sample : M3953-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-RR-03-(SA)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.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
Butane, 2-metho...	2.175	102.5	ng	5991600	1	6.886	1169270	20.0
Ethanol, 2-(2-b...	8.063	2.5	ng	205261	2	8.169	1632160	20.0
2(3H)-Benzothia...	10.798	2.3	ng	198447	4	11.404	1706410	20.0
n-Hexadecanoic ...	11.927	8.3	ng	710713	4	11.404	1706410	20.0
Octadecanoic acid	12.715	3.2	ng	275481	4	11.404	1706410	20.0
Octacosane	13.262	3.4	ng	299135	5	14.039	1771960	20.0
1-Hexacosene	13.892	2.1	ng	182814	5	14.039	1771960	20.0
Octacosane, 2-m...	14.439	3.4	ng	304637	5	14.039	1771960	20.0
unknown14.862	14.862	4.3	ng	237396	6	15.515	1106890	20.0
Eicosane	15.345	4.7	ng	258910	6	15.515	1106890	20.0
Dotriacontane, ...	16.409	2.8	ng	152459	6	15.515	1106890	20.0
Methyl 3beta-ac...	17.386	10.8	ng	598165	6	15.515	1106890	20.0