

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051023\
 Data File : BF133329.D
 Acq On : 10 May 2023 14:24
 Operator : CG\JU
 Sample : 02719-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-04_10-12_20230509

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133329.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.263	365	370	376	rBV	77549	96564	1.97%	0.206%
2	4.916	475	481	496	rBV	1054649	1413201	28.79%	3.010%
3	5.340	549	553	573	rBV	4091194	4500459	91.70%	9.585%
4	5.728	616	619	625	rBV	150094	140823	2.87%	0.300%
5	6.369	723	728	731	rBV	4094340	4452083	90.71%	9.482%
6	6.722	785	788	791	rBV	1617281	1217396	24.80%	2.593%
7	7.286	880	884	887	rBV	3105757	2941258	59.93%	6.264%
8	8.004	1003	1006	1010	rBV	1903692	1653871	33.70%	3.522%
9	9.086	1186	1190	1193	rBV	5488920	4907955	100.00%	10.453%
10	9.757	1301	1304	1308	rBV	2267776	1838913	37.47%	3.916%
11	10.469	1422	1425	1429	rBV	426449	329672	6.72%	0.702%
12	10.545	1434	1438	1442	rBV	2161005	1965736	40.05%	4.186%
13	11.198	1546	1549	1553	rVB3	81274	88252	1.80%	0.188%
14	11.239	1553	1556	1560	rBV	2112801	1796470	36.60%	3.826%
15	11.633	1620	1623	1627	rBV2	80587	105936	2.16%	0.226%
16	11.774	1638	1647	1668	rVB	2363544	4435744	90.38%	9.447%
17	12.039	1689	1692	1698	rVB	197294	265812	5.42%	0.566%
18	12.357	1744	1746	1751	rBV3	59846	81663	1.66%	0.174%
19	12.421	1755	1757	1761	rVV	114664	178917	3.65%	0.381%
20	12.474	1761	1766	1772	rVV8	175617	559536	11.40%	1.192%
21	12.557	1773	1780	1792	rVB	2197107	3741419	76.23%	7.968%
22	12.827	1822	1826	1830	rBV	4468116	4385930	89.36%	9.341%
23	13.380	1916	1920	1923	rBV2	137871	218432	4.45%	0.465%
24	13.745	1978	1982	1991	rVB3	280893	499808	10.18%	1.064%
25	13.874	2001	2004	2007	rBV	1240978	1209529	24.64%	2.576%
26	13.910	2007	2010	2016	rVB	313150	422312	8.60%	0.899%
27	14.051	2032	2034	2038	rVB	127565	117728	2.40%	0.251%
28	14.368	2084	2088	2096	rVB	415170	702343	14.31%	1.496%
29	14.657	2134	2137	2140	rVB	186928	200440	4.08%	0.427%
30	14.810	2159	2163	2171	rBV	400236	618645	12.60%	1.318%
31	14.974	2189	2191	2195	rVB	202791	205952	4.20%	0.439%
32	15.298	2242	2246	2251	rBV	1275052	1661629	33.86%	3.539%

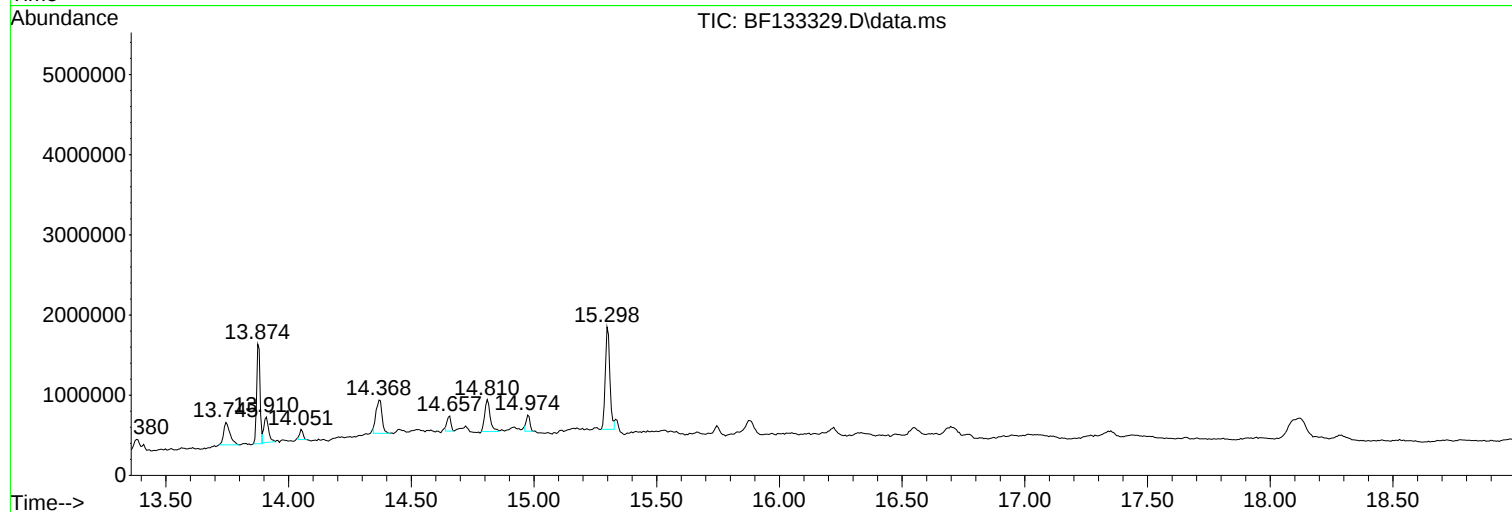
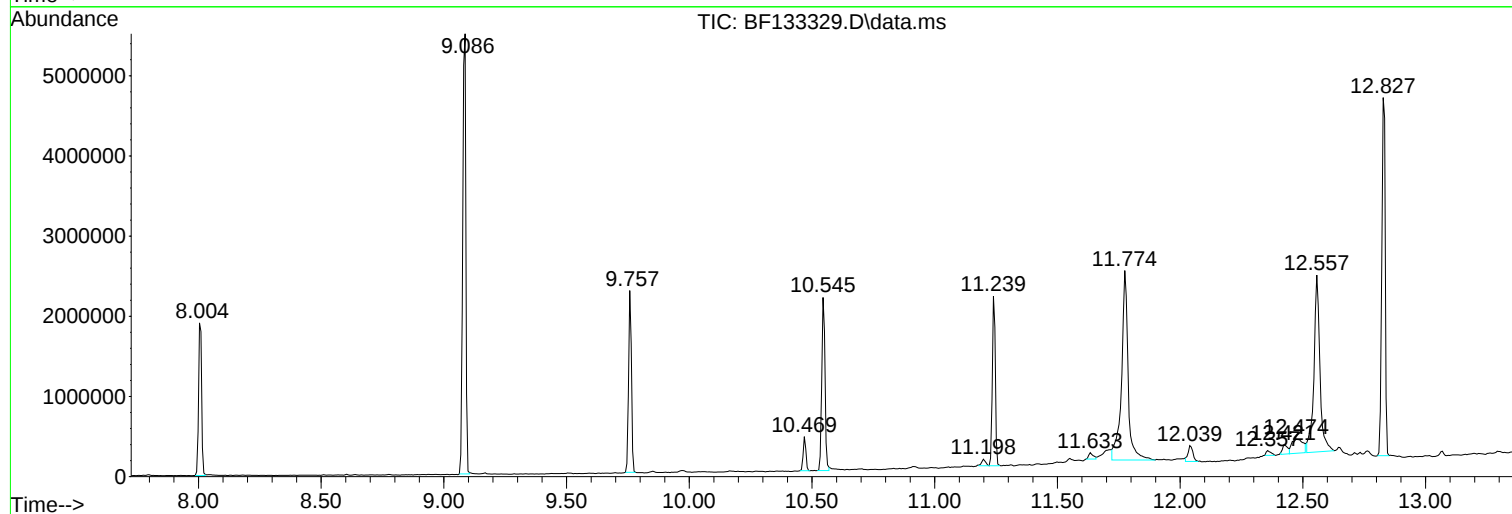
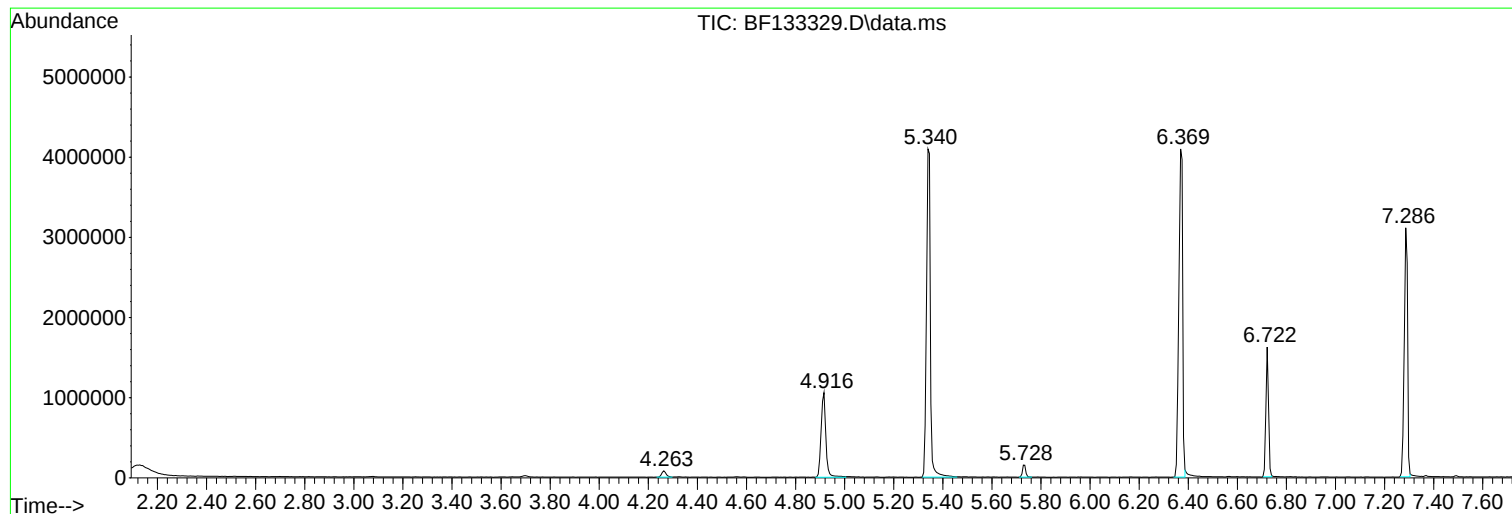
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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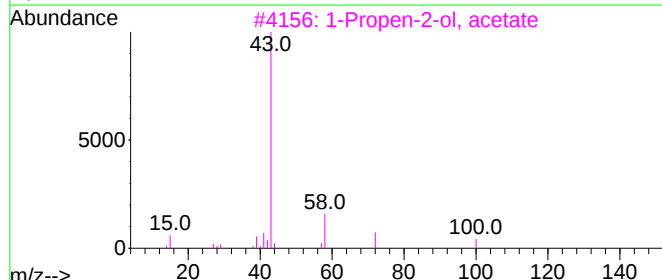
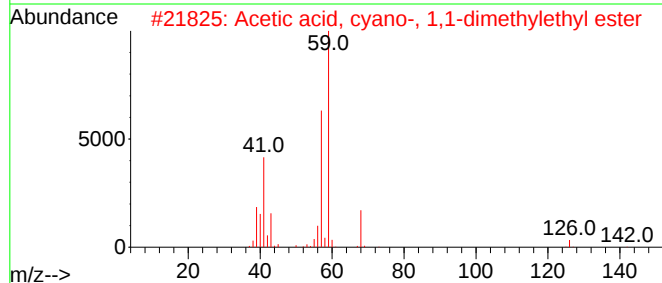
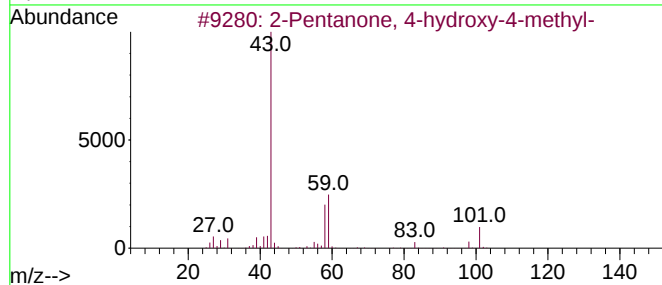
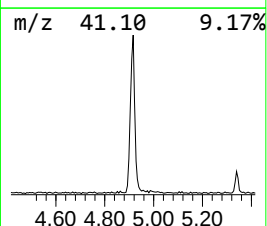
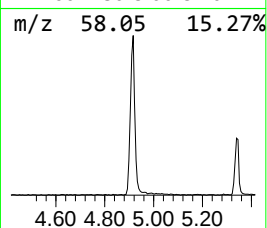
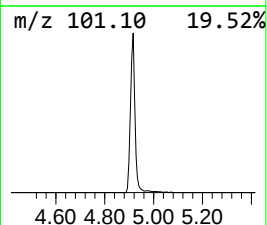
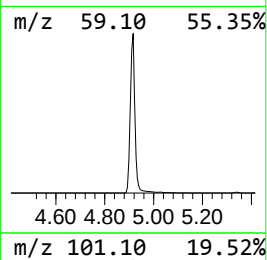
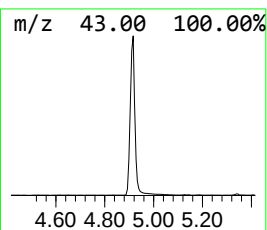
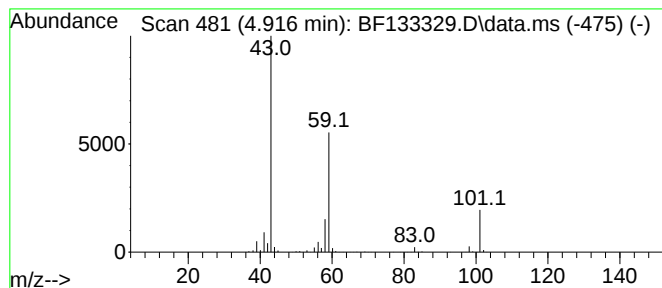
Instrument :
BNA_F
ClientSampleId :
SB-04_10-12_20230509

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.916	23.22 ng	1413200	1,4-Dichlorobenzene-d4	6.722	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9



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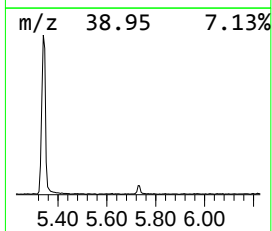
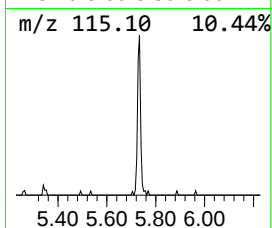
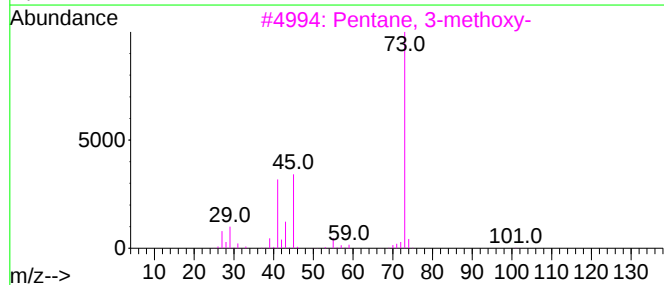
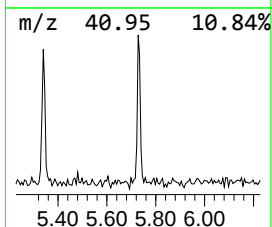
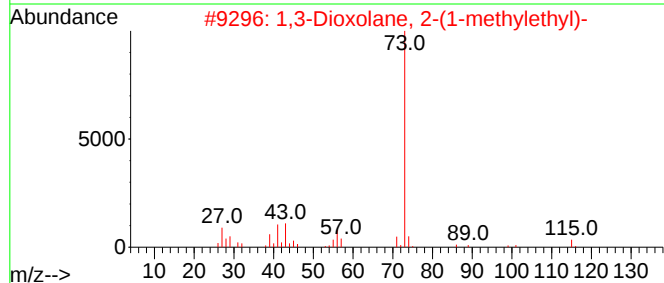
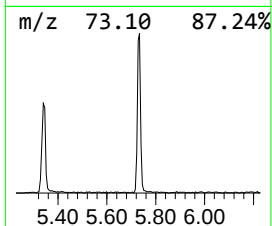
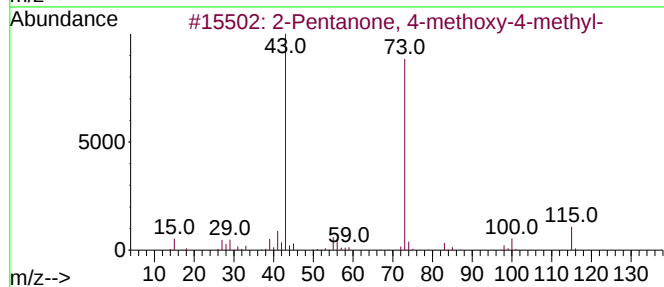
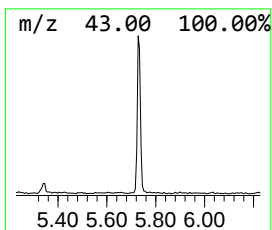
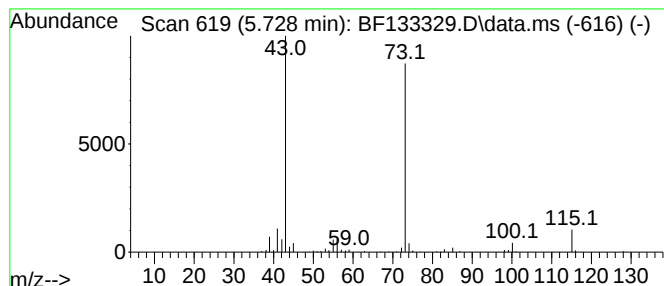
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.728	2.31 ng	140823	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	25
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	12



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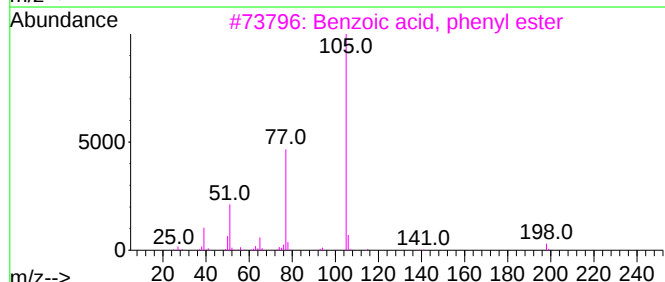
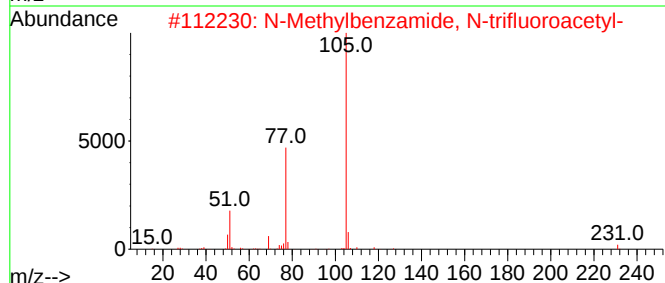
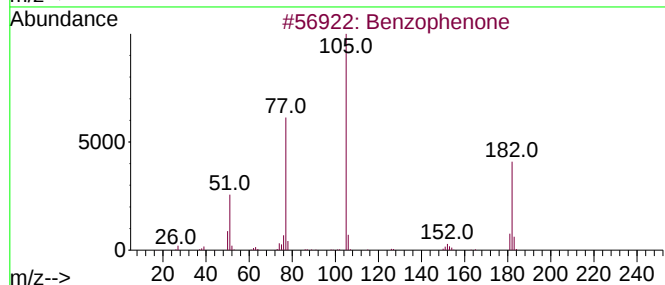
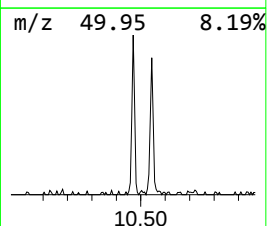
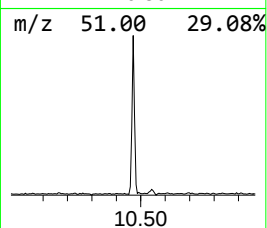
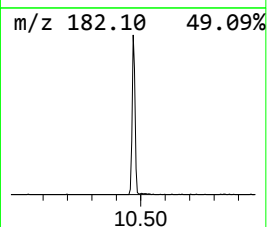
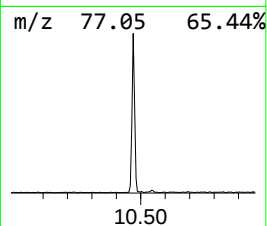
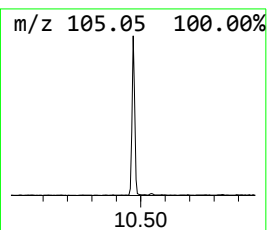
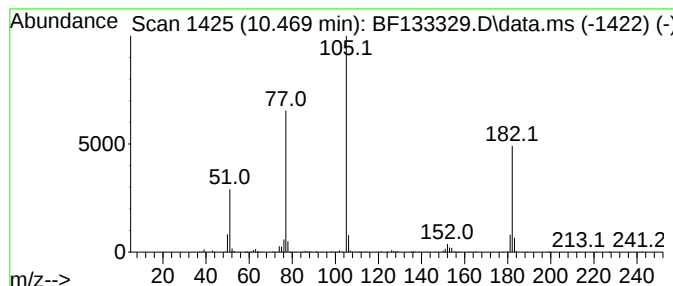
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	3.59 ng	329672	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
3			Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
5			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47



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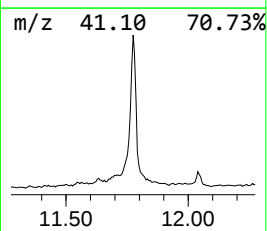
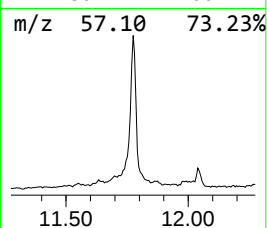
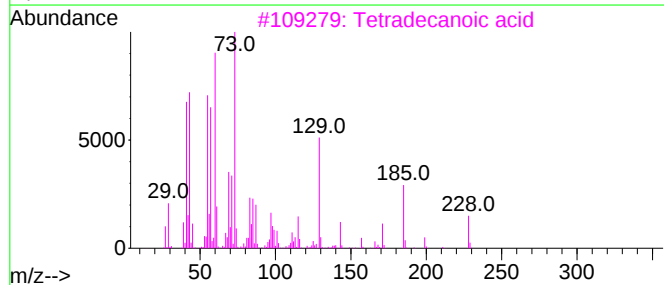
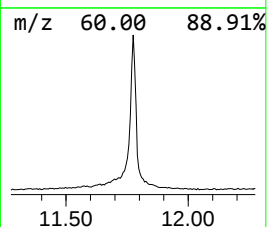
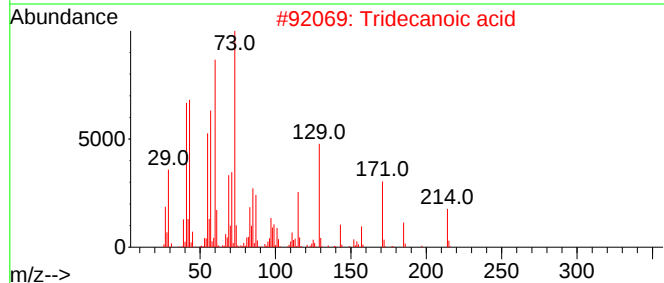
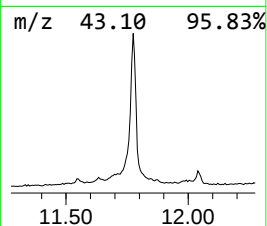
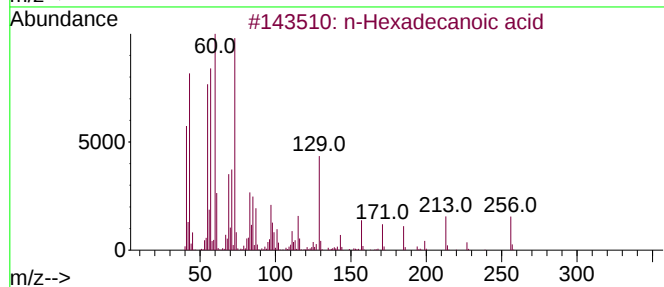
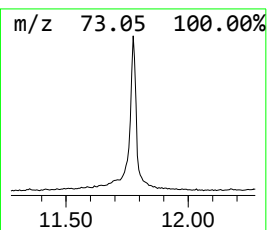
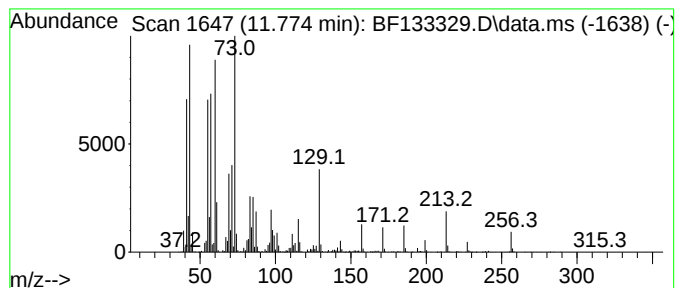
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.774	49.38 ng	4435740	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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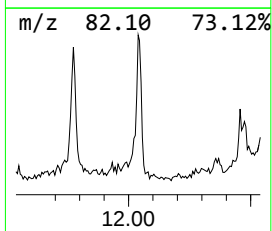
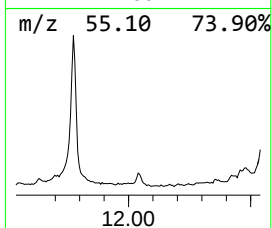
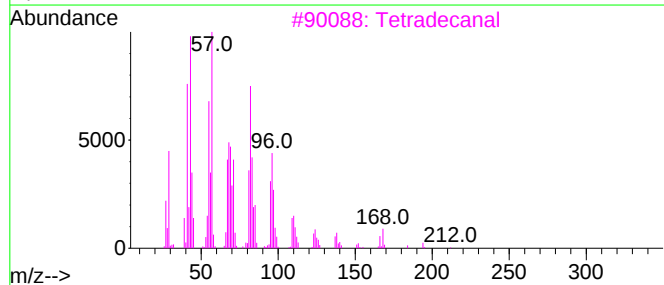
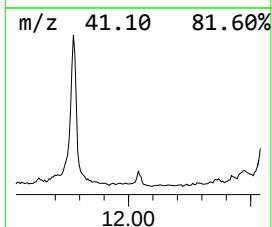
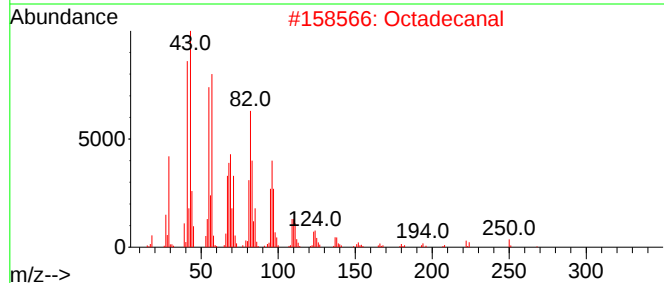
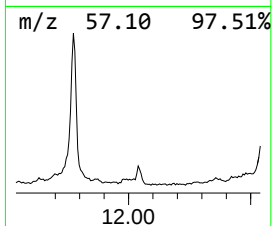
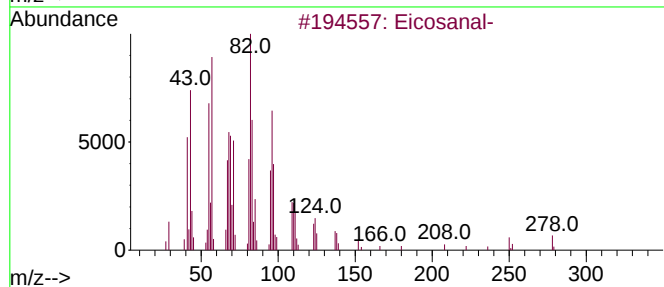
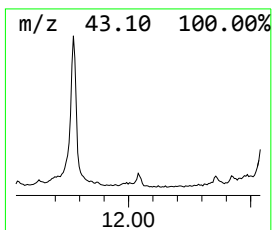
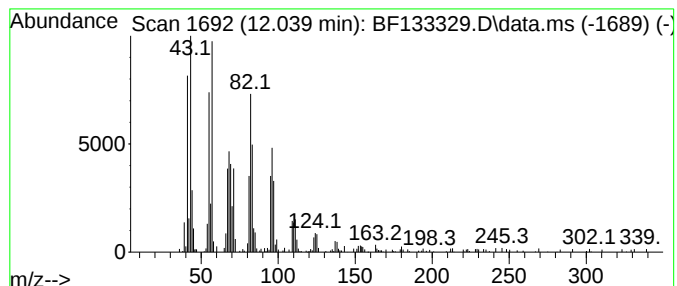
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Eicosanal- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.039	2.96 ng	265812	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosanal-	296	C20H40O	002400-66-0	94
2			Octadecanal	268	C18H36O	000638-66-4	91
3			Tetradecanal	212	C14H28O	000124-25-4	91
4			Pentadecanal-	226	C15H30O	002765-11-9	91
5			Tetracosanal	352	C24H48O	057866-08-7	91



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ALS Vial : 5 Sample Multiplier: 1

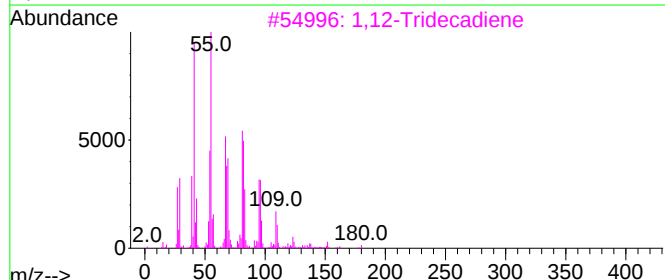
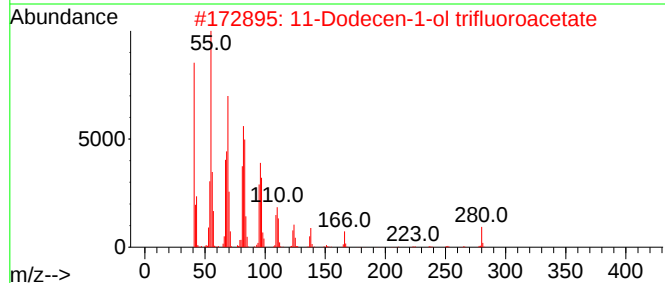
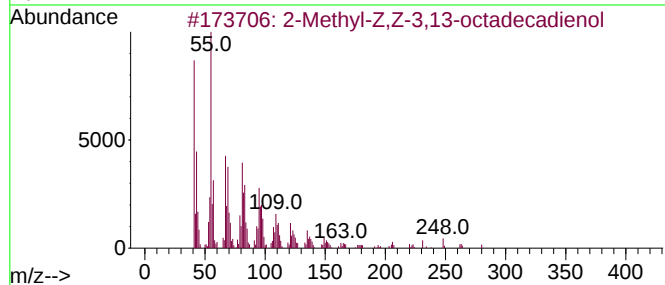
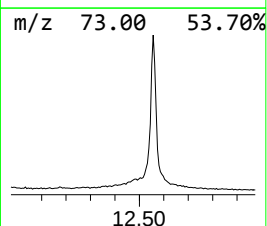
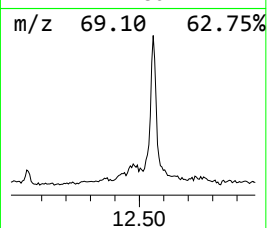
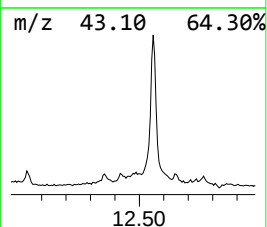
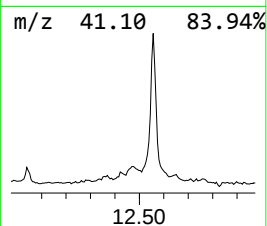
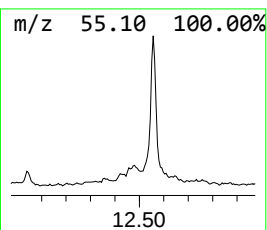
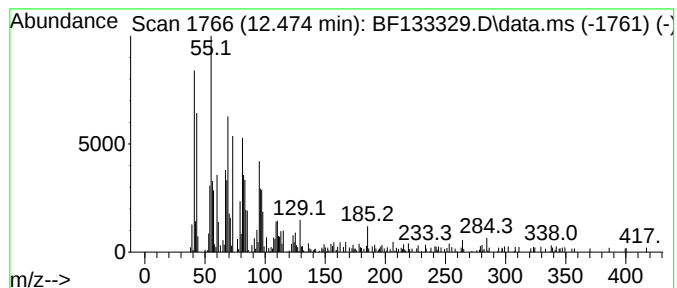
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Methyl-Z,Z-3,13-octadecad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.474	6.23 ng	559536	Phenanthrene-d10	11.239	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-Z,Z-3,13-octadecadienol	280	C19H36O	1000130-90-5	83
2	11-Dodecen-1-ol trifluoroacetate	280	C14H23F3O2	128792-46-1	62
3	1,12-Tridecadiene	180	C13H24	021964-48-7	60
4	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	60
5	Oleic Acid	282	C18H34O2	000112-80-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051023\
Data File : BF133329.D
Acq On : 10 May 2023 14:24
Operator : CG\JU
Sample : 02719-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-04_10-12_20230509

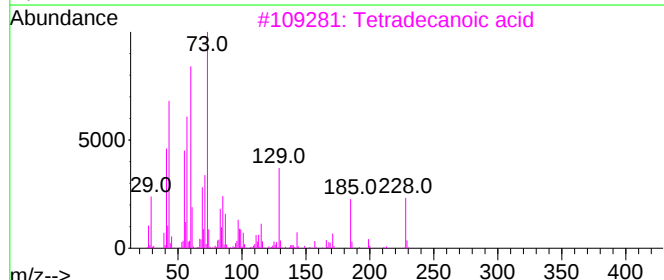
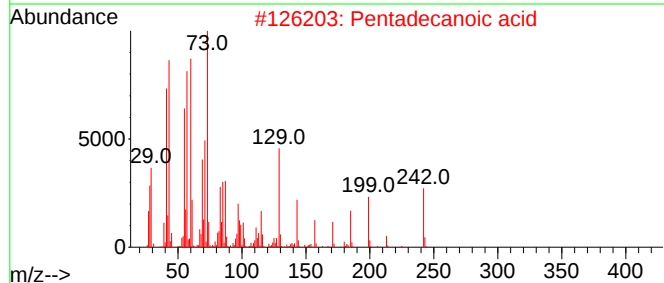
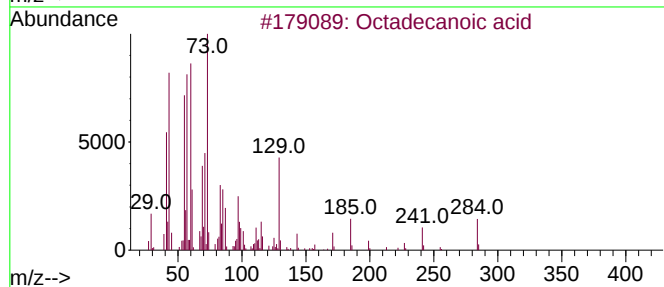
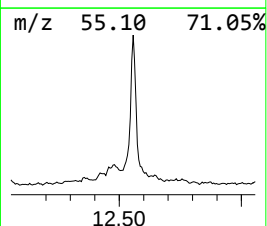
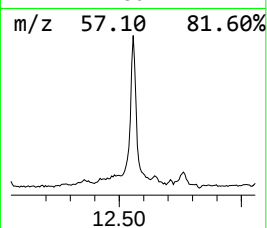
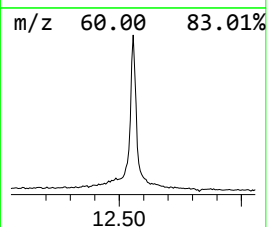
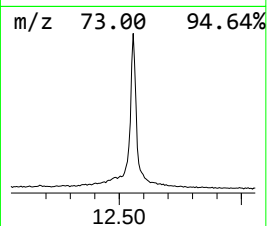
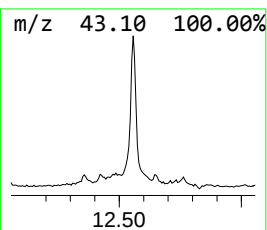
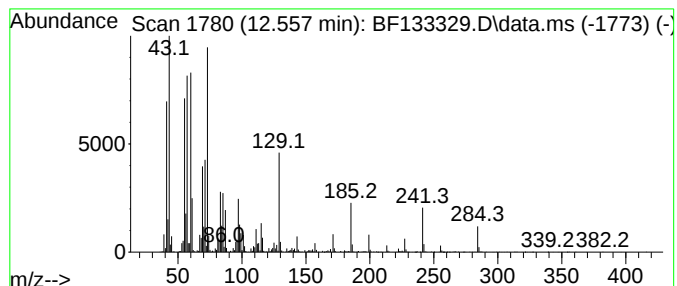
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.557	61.87 ng	3741420	Chrysene-d12	13.874

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	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051023\
Data File : BF133329.D
Acq On : 10 May 2023 14:24
Operator : CG\JU
Sample : 02719-04
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Instrument :
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ClientSampleId :
SB-04_10-12_20230509

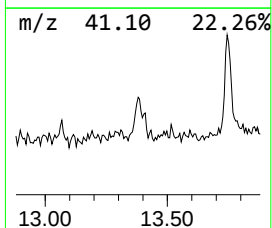
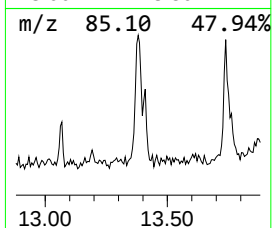
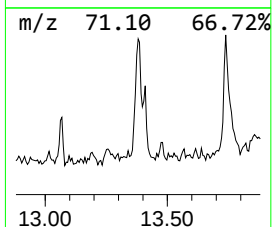
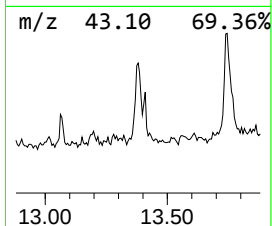
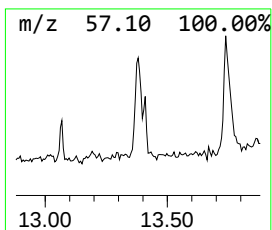
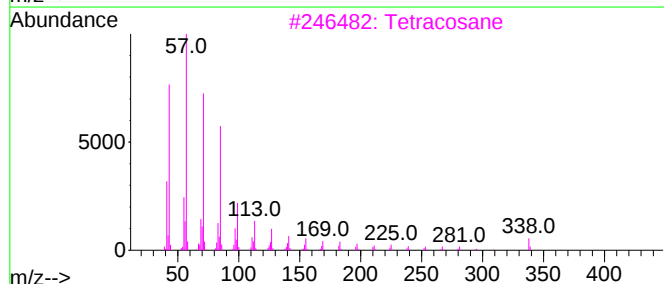
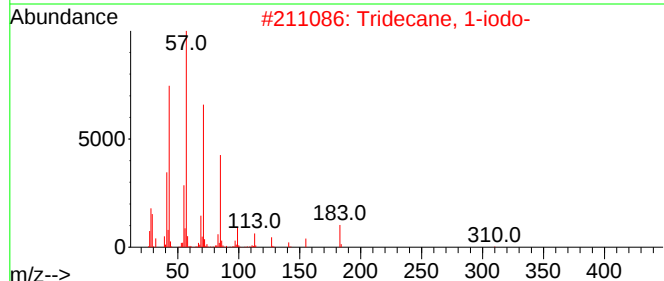
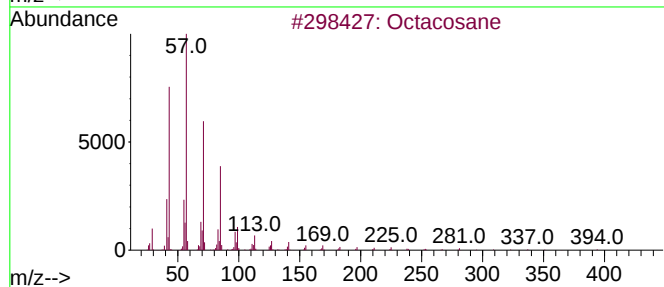
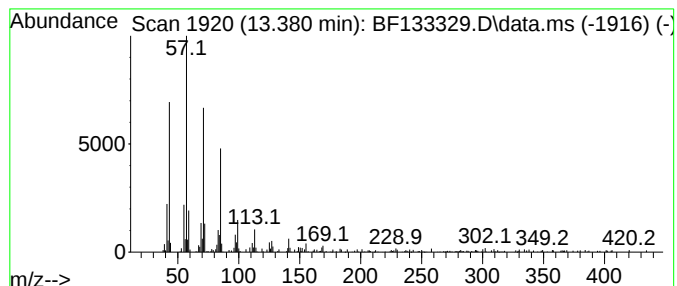
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.380	3.61 ng	218432	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	97
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	96
3			Tetracosane	338	C24H50	000646-31-1	93
4			Heneicosane	296	C21H44	000629-94-7	89
5			Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051023\
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Acq On : 10 May 2023 14:24
Operator : CG\JU
Sample : 02719-04
Misc :
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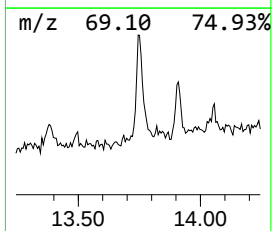
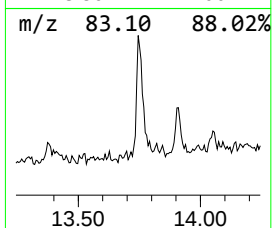
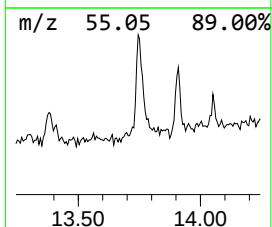
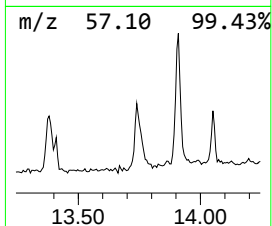
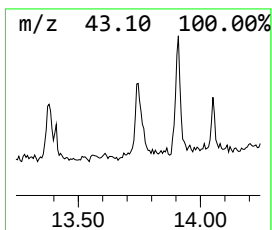
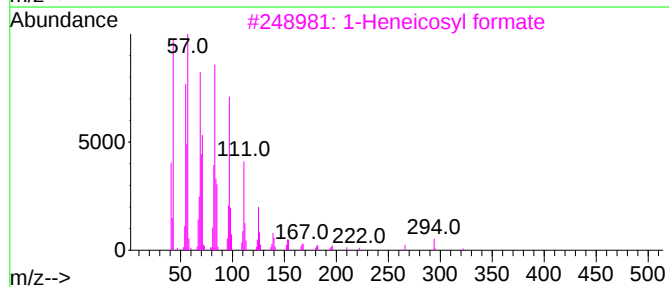
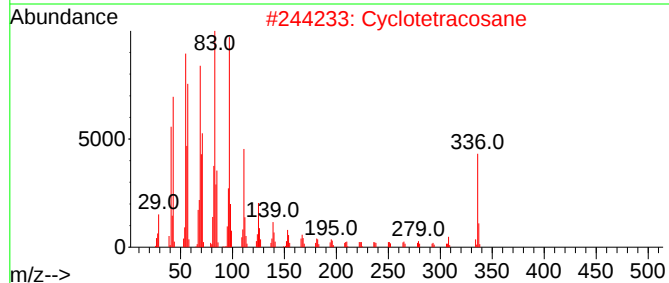
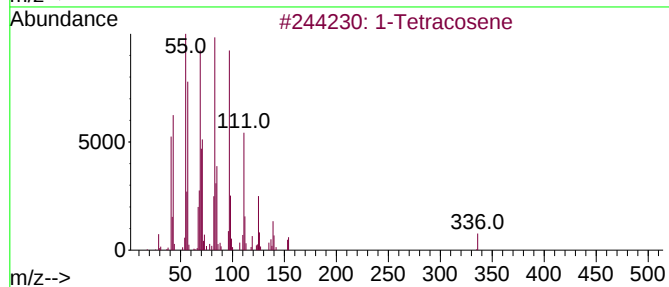
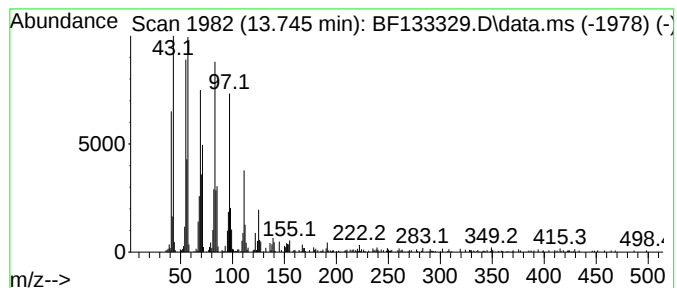
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Tetracosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.745	8.26 ng	499808	Chrysene-d12	13.874	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	99
2	Cyclotetracosane	336	C24H48	000297-03-0	95
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
4	1-Docosene	308	C22H44	001599-67-3	95
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051023\
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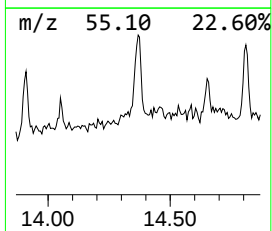
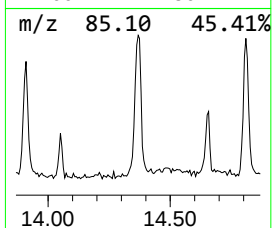
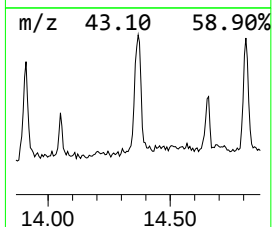
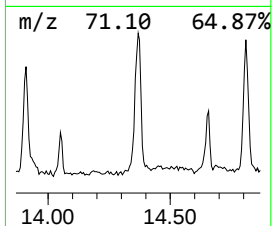
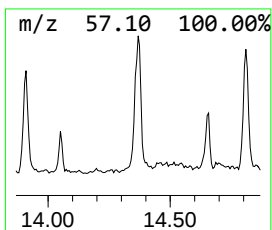
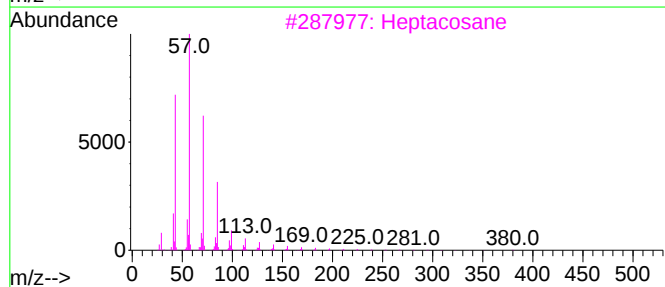
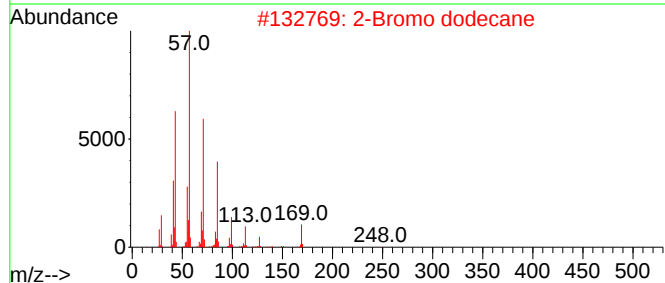
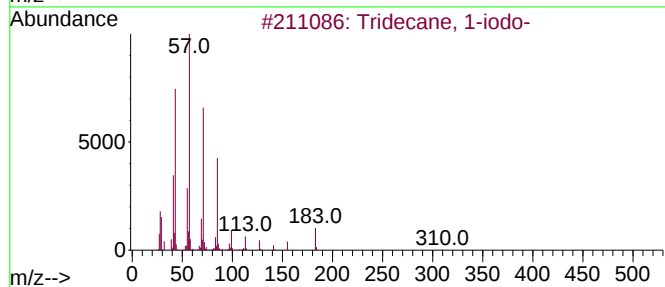
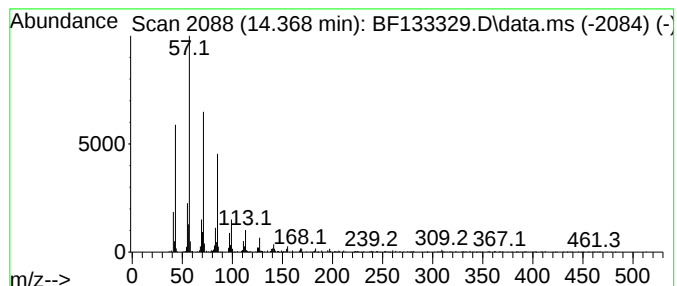
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tridecane, 1-iodo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.368	11.61 ng	702343	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
2			2-Bromo dodecane	248	C12H25Br	013187-99-0	93
3			Heptacosane	380	C27H56	000593-49-7	90
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5			Tridecane, 6-propyl-	226	C16H34	055045-10-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051023\
Data File : BF133329.D
Acq On : 10 May 2023 14:24
Operator : CG\JU
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ALS Vial : 5 Sample Multiplier: 1

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ClientSampleId :
SB-04_10-12_20230509

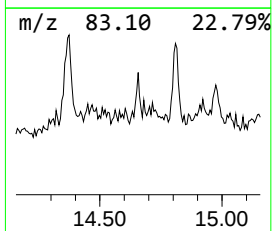
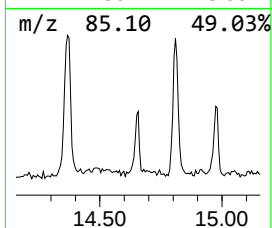
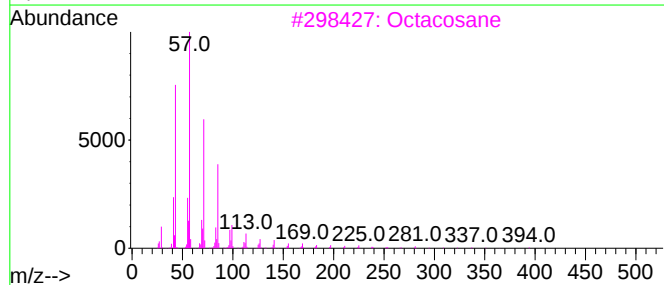
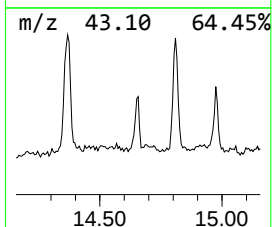
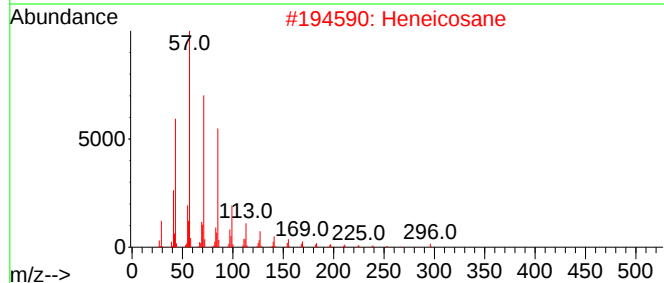
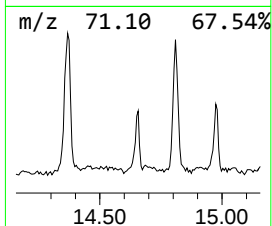
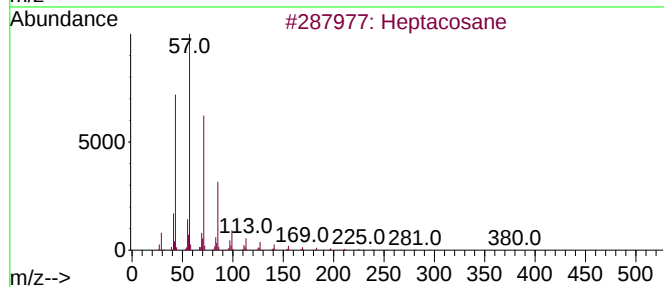
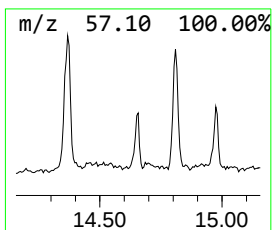
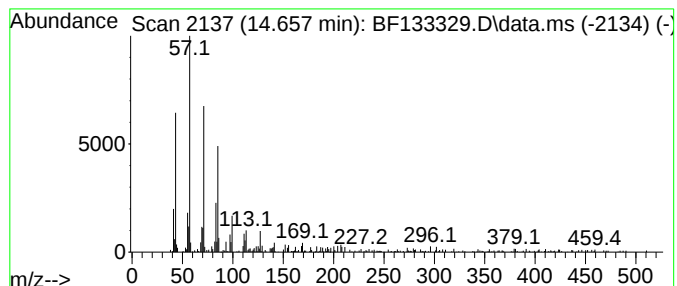
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.657	2.41 ng	200440	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	95
2			Heneicosane	296	C21H44	000629-94-7	95
3			Octacosane	394	C28H58	000630-02-4	93
4			Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	81
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051023\
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ALS Vial : 5 Sample Multiplier: 1

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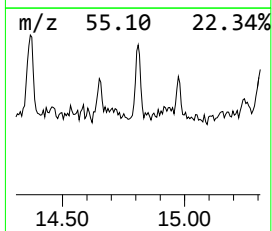
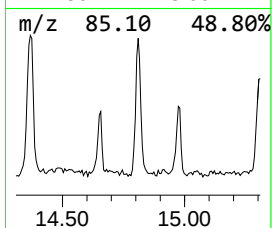
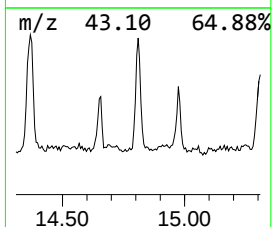
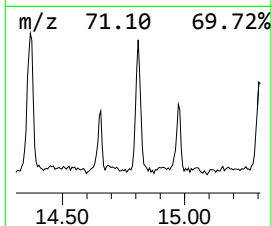
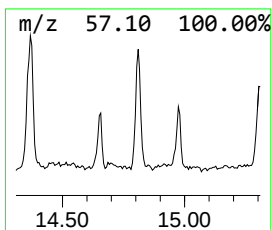
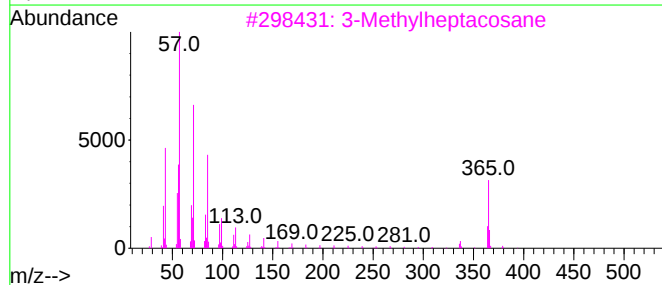
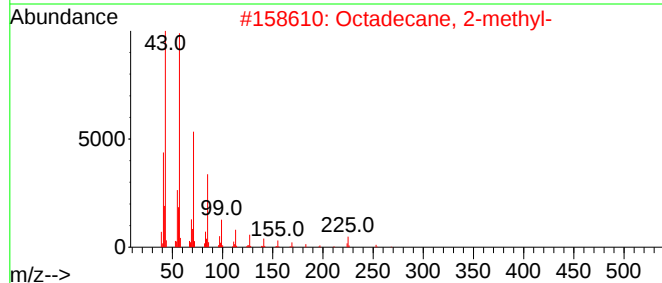
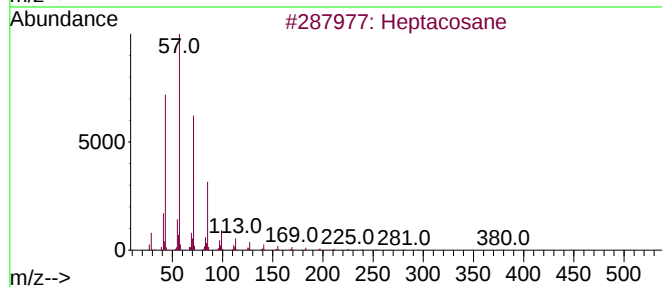
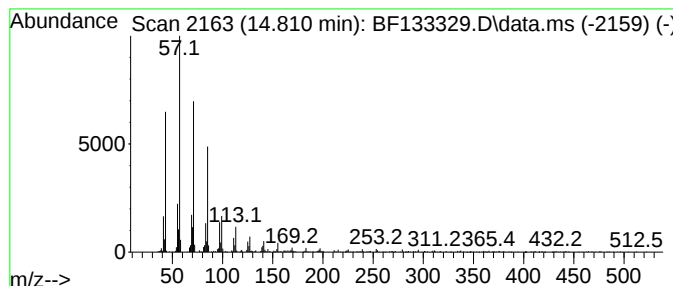
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	7.45 ng	618645	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	94
2			Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
3			3-Methylheptacosane	394	C28H58	014167-66-9	93
4			Dotriacontane, 2-methyl-	465	C33H68	001720-11-2	92
5			Octadecane	254	C18H38	000593-45-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051023\
Data File : BF133329.D
Acq On : 10 May 2023 14:24
Operator : CG\JU
Sample : 02719-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04_10-12_20230509

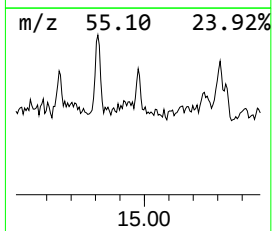
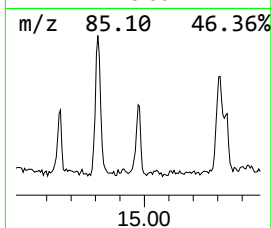
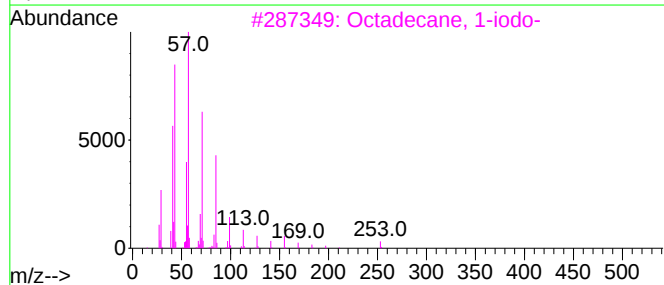
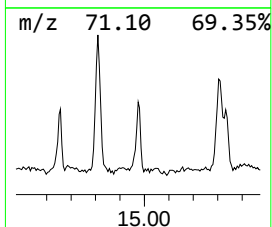
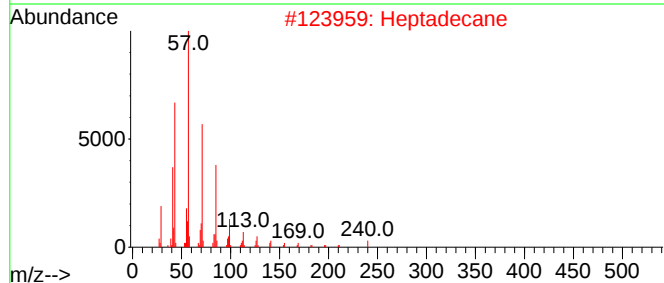
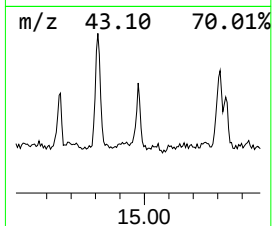
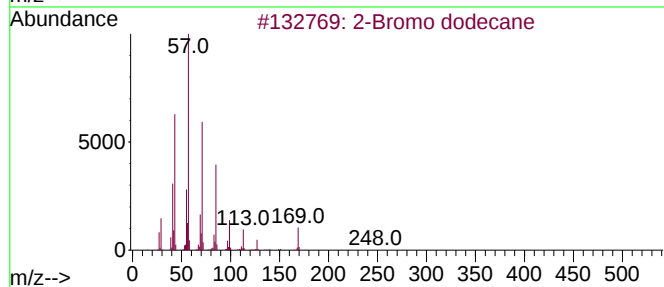
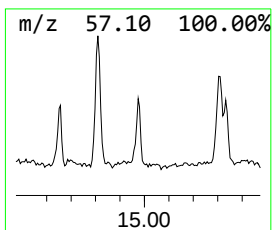
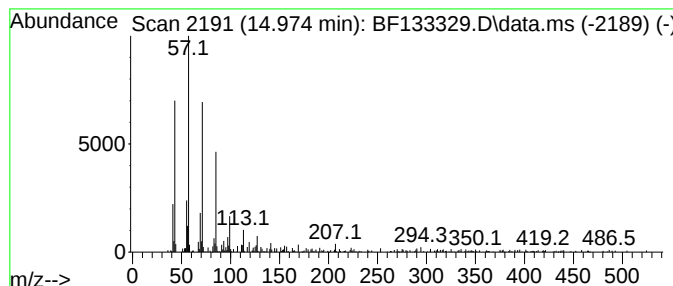
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2-Bromo dodecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	2.48 ng	205952	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2			Heptadecane	240	C17H36	000629-78-7	90
3			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
4			Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051023\
Data File : BF133329.D
Acq On : 10 May 2023 14:24
Operator : CG\JU
Sample : 02719-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04_10-12_20230509

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
2-Pentanone, 4-...	4.916	23.2	ng	1413200	1	6.722	1217400	20.0
2-Pentanone, 4-...	5.728	2.3	ng	140823	1	6.722	1217400	20.0
Benzophenone	10.469	3.6	ng	329672	3	9.757	1838910	20.0
n-Hexadecanoic ...	11.774	49.4	ng	4435740	4	11.239	1796470	20.0
Eicosanal-	12.039	3.0	ng	265812	4	11.239	1796470	20.0
2-Methyl-Z,Z-3,...	12.474	6.2	ng	559536	4	11.239	1796470	20.0
Octadecanoic acid	12.557	61.9	ng	3741420	5	13.874	1209530	20.0
Octacosane	13.380	3.6	ng	218432	5	13.874	1209530	20.0
1-Tetracosene	13.745	8.3	ng	499808	5	13.874	1209530	20.0
Tridecane, 1-iodo-	14.368	11.6	ng	702343	5	13.874	1209530	20.0
Heptacosane	14.657	2.4	ng	200440	6	15.298	1661630	20.0
Octadecane, 2-m...	14.810	7.5	ng	618645	6	15.298	1661630	20.0
2-Bromo dodecane	14.974	2.5	ng	205952	6	15.298	1661630	20.0