

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092623\
 Data File : BF135450.D
 Acq On : 26 Sep 2023 13:50
 Operator : CG\JU
 Sample : 04566-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CPT102-06

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135450.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.393	558	562	584	rBV	3589168	3596673	94.15%	12.971%
2	6.404	729	734	749	rBV	3618785	3820249	100.00%	13.777%
3	6.604	763	768	781	rBV	39356	104549	2.74%	0.377%
4	6.751	790	793	797	rBV	1160508	963315	25.22%	3.474%
5	7.316	885	889	893	rBV	2410724	2433055	63.69%	8.774%
6	8.034	1006	1011	1014	rBV	1377819	1258605	32.95%	4.539%
7	9.110	1189	1194	1197	rBV	3956165	3727090	97.56%	13.441%
8	9.234	1209	1215	1224	rVB	599478	675515	17.68%	2.436%
9	9.786	1305	1309	1313	rBV	1556223	1316687	34.47%	4.748%
10	9.998	1339	1345	1355	rBV3	41220	73262	1.92%	0.264%
11	10.586	1440	1445	1448	rBV	2185699	2194410	57.44%	7.914%
12	10.645	1453	1455	1463	rVB	69189	80221	2.10%	0.289%
13	10.951	1502	1507	1512	rBV6	28200	45783	1.20%	0.165%
14	11.280	1559	1563	1566	rBV	1527425	1282779	33.58%	4.626%
15	11.304	1566	1567	1570	rVV	115891	75932	1.99%	0.274%
16	11.351	1572	1575	1580	rVB2	30980	42999	1.13%	0.155%
17	11.816	1646	1654	1666	rBV2	555240	726606	19.02%	2.620%
18	12.386	1746	1751	1756	rBV7	29265	47156	1.23%	0.170%
19	12.504	1768	1771	1774	rBV	72660	88611	2.32%	0.320%
20	12.604	1783	1788	1800	rVB	190925	293067	7.67%	1.057%
21	12.733	1807	1810	1816	rVB	50034	57108	1.49%	0.206%
22	12.874	1830	1834	1838	rBV	2596787	2467674	64.59%	8.899%
23	13.363	1912	1917	1922	rBV	79910	91411	2.39%	0.330%
24	13.651	1962	1966	1971	rBV2	44322	85355	2.23%	0.308%
25	13.869	1998	2003	2009	rBV6	43212	112393	2.94%	0.405%
26	13.939	2011	2015	2024	rVB	803331	809890	21.20%	2.921%
27	14.410	2092	2095	2098	rBV	41408	38204	1.00%	0.138%
28	14.786	2156	2159	2163	rVB	37456	40067	1.05%	0.144%
29	15.051	2200	2204	2209	rBV	87967	153825	4.03%	0.555%
30	15.404	2259	2264	2273	rBV	808197	1026755	26.88%	3.703%

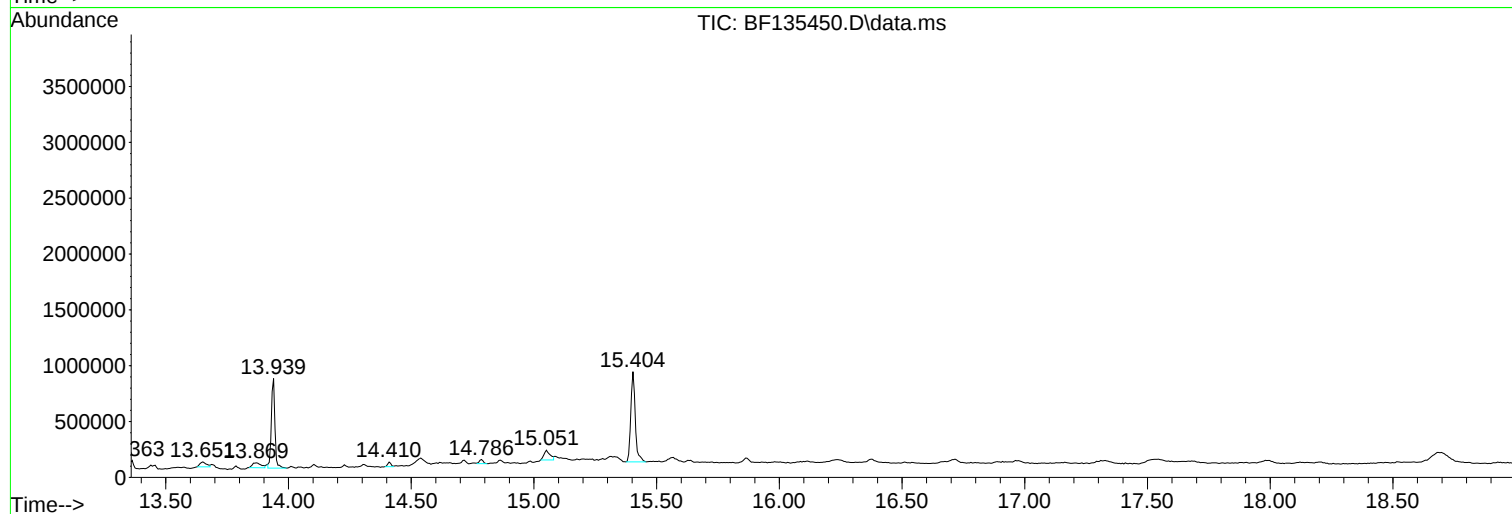
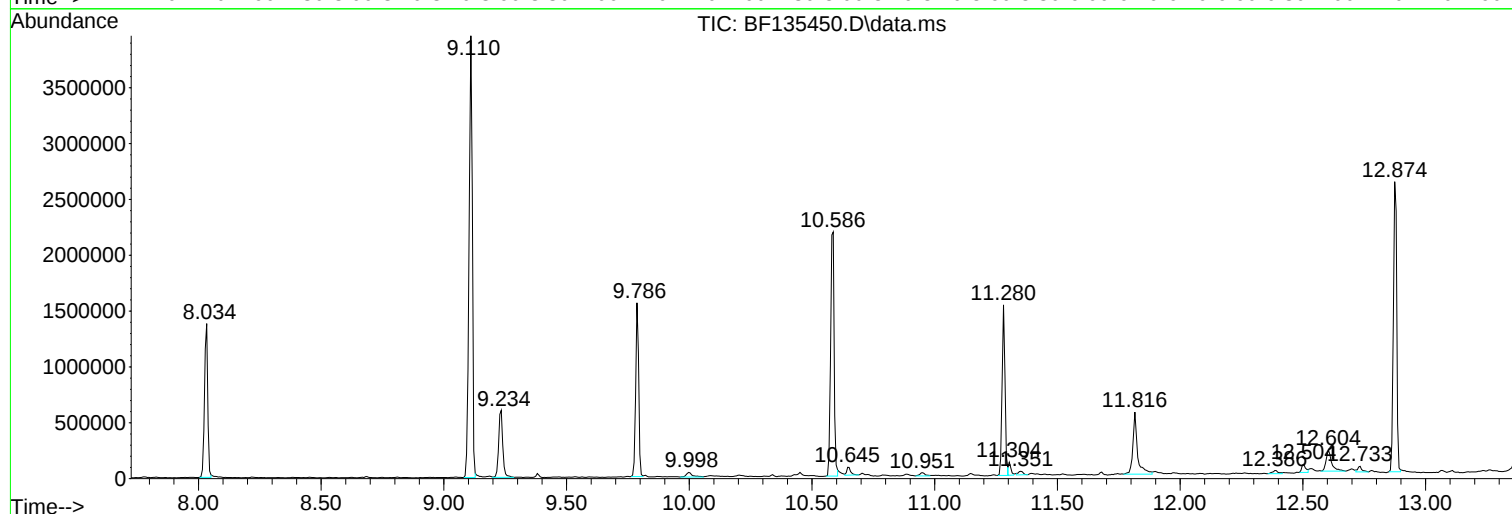
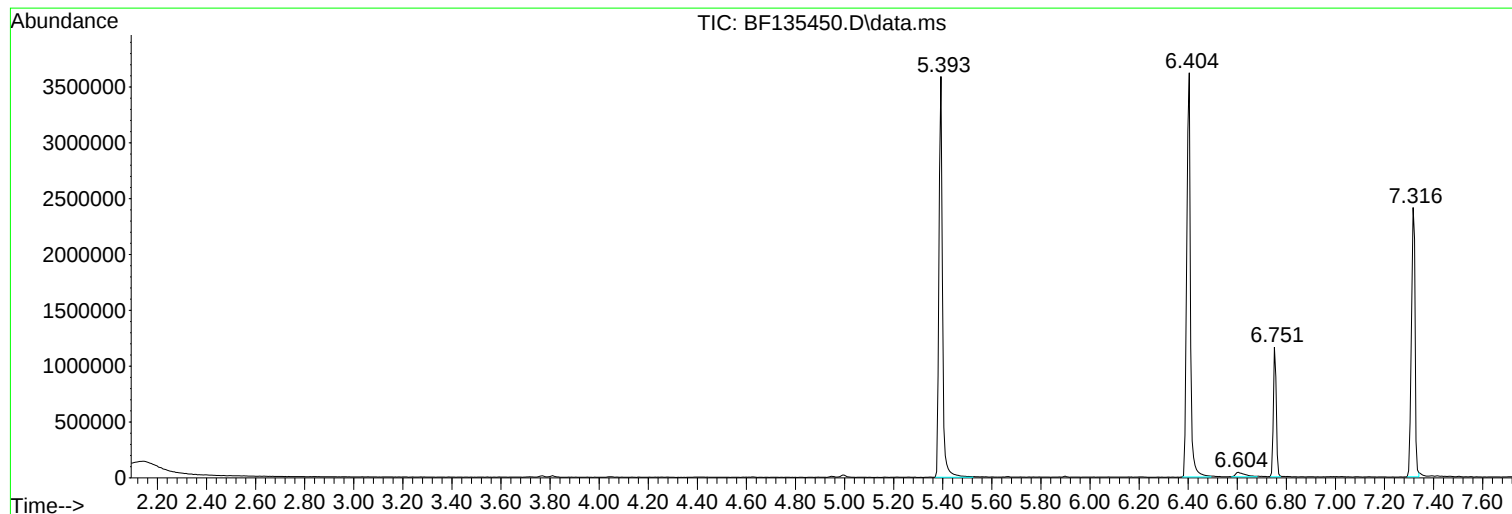
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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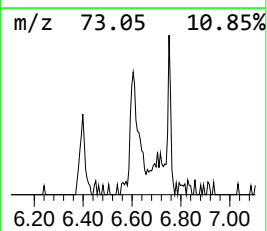
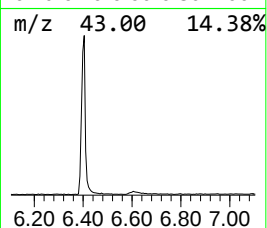
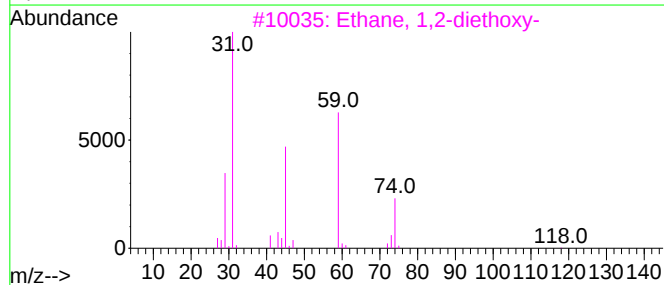
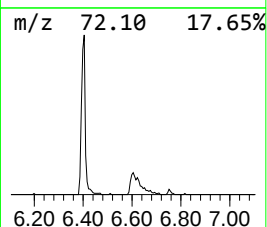
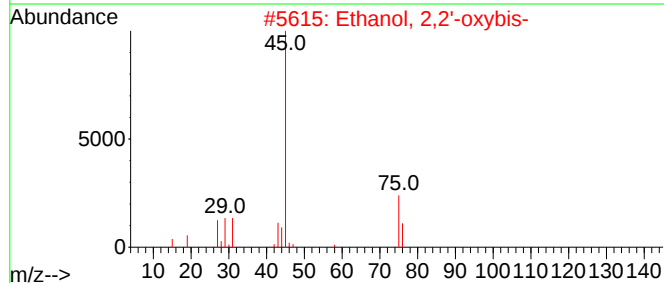
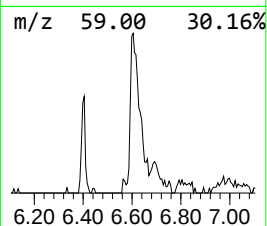
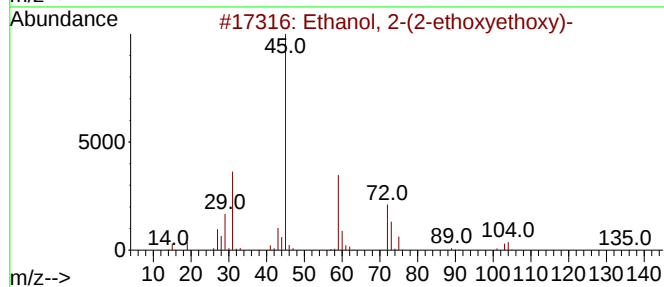
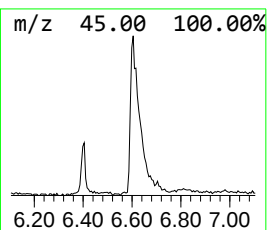
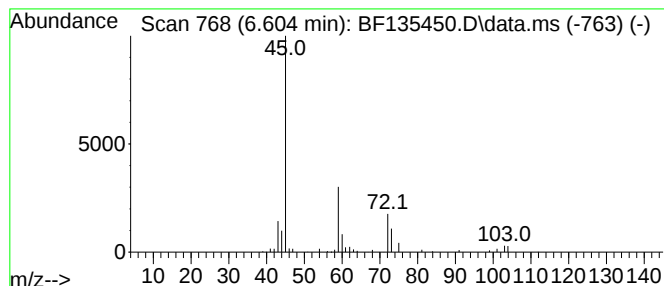
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.604	2.17 ng	104549	1,4-Dichlorobenzene-d4	6.751

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	78
2			Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	40
3			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	38
4			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	37
5			Methoxyacetic acid, 2-methylprop...	146	C7H14O3	1000282-40-9	28



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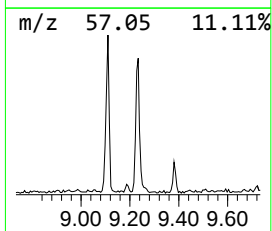
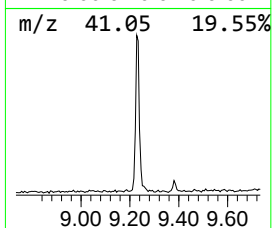
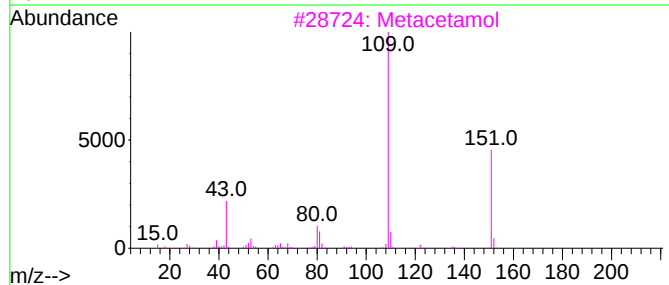
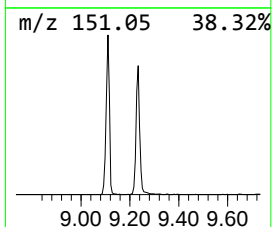
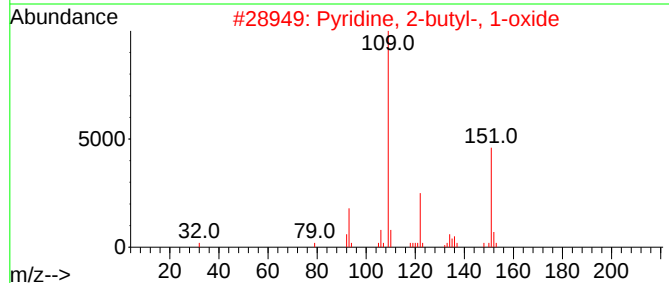
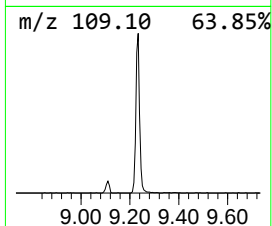
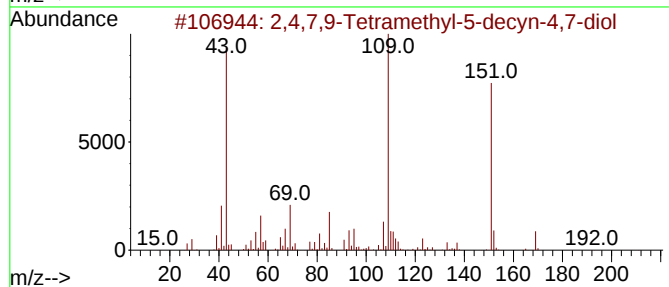
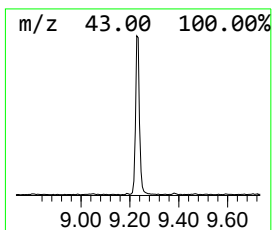
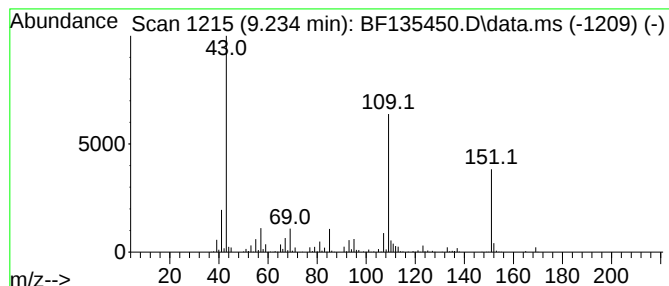
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.234	10.26 ng	675515	Acenaphthene-d10			9.786

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO		031396-32-4	59
3	Metacetamol	151	C8H9NO2		000621-42-1	53
4	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O		000116-02-9	38
5	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3		1000107-08-7	36



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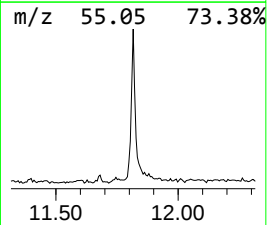
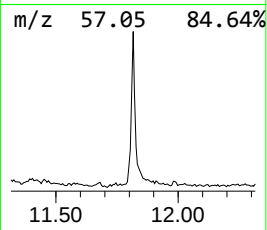
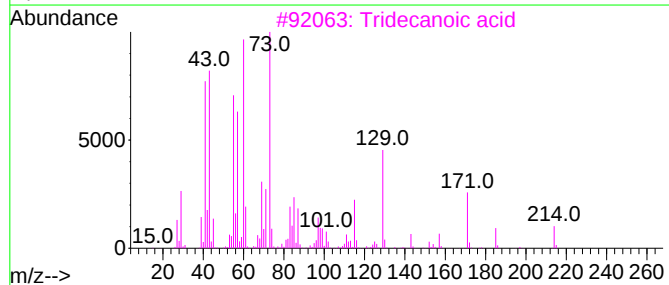
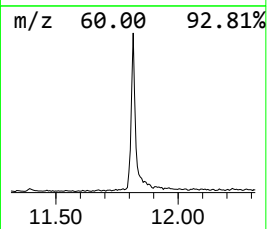
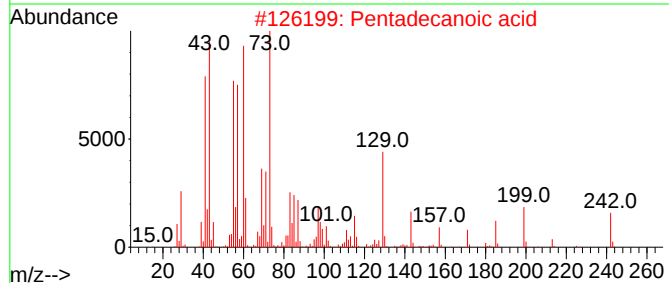
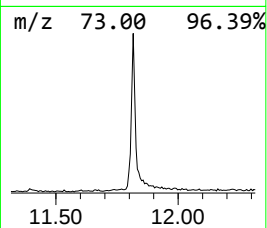
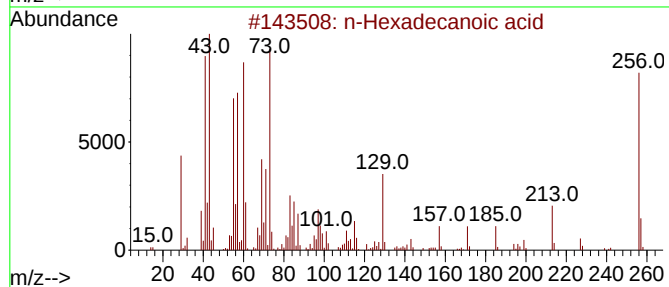
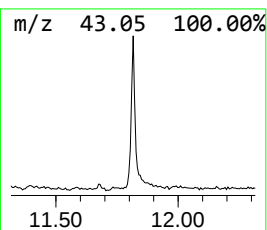
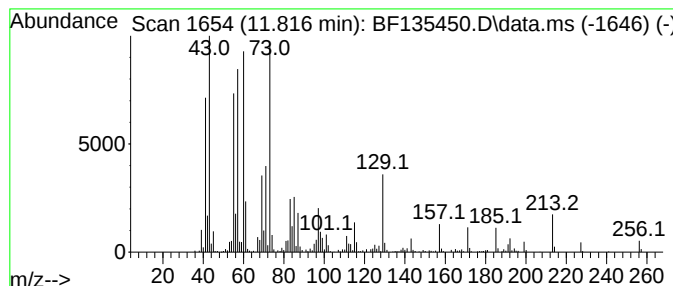
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	11.33 ng	726606	Phenanthrene-d10	11.281

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	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	83



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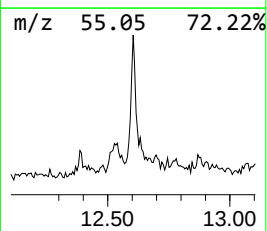
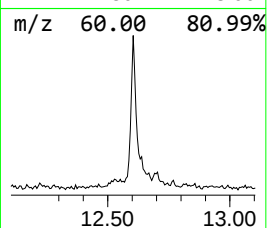
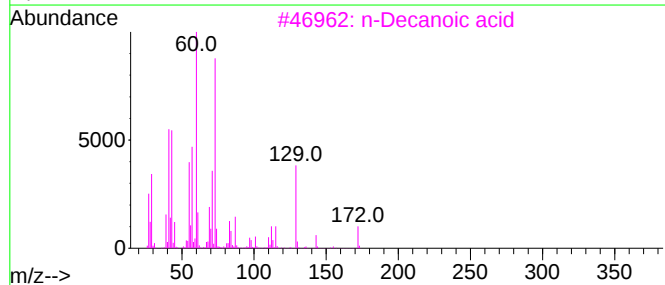
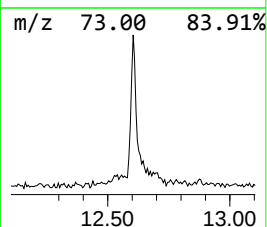
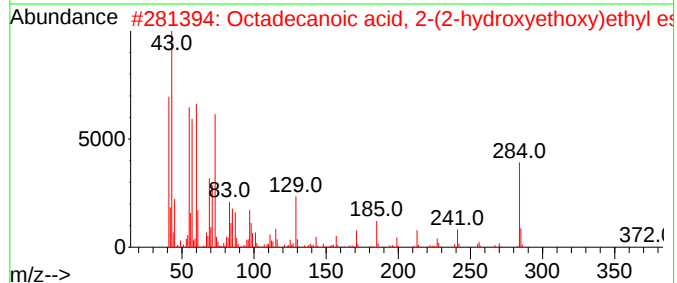
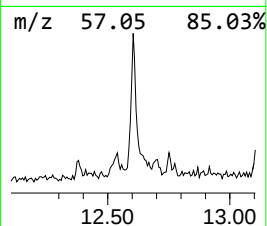
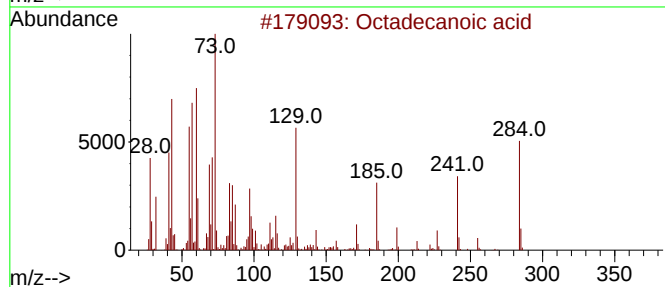
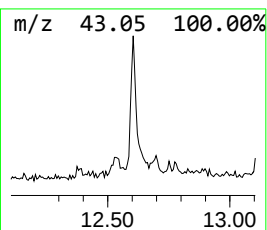
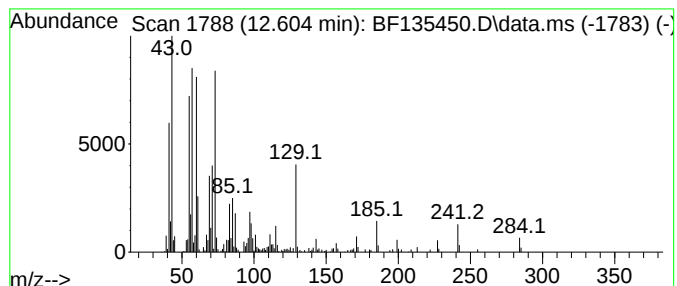
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.604	4.57 ng	293067	Phenanthrene-d10	11.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
3			n-Decanoic acid	172	C10H20O2	000334-48-5	68
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	49



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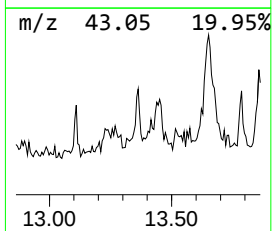
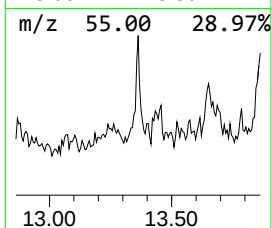
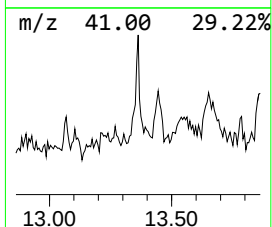
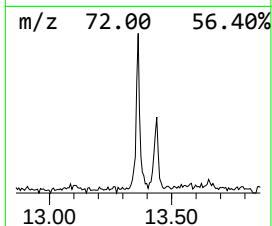
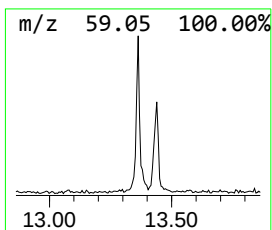
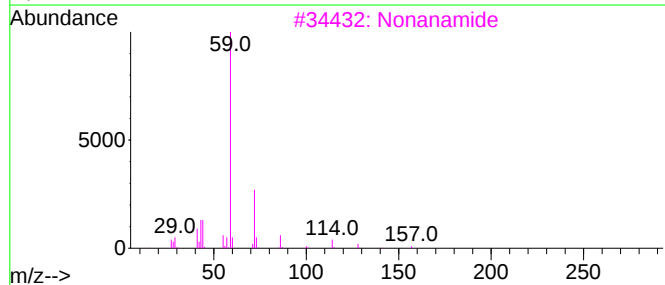
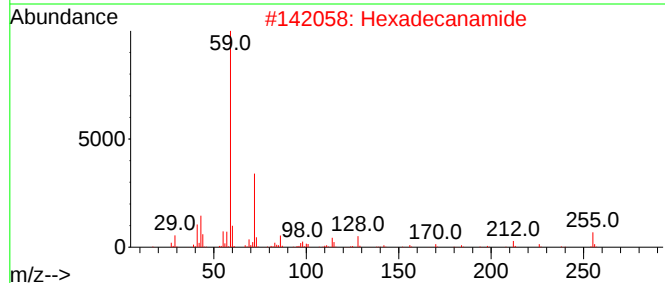
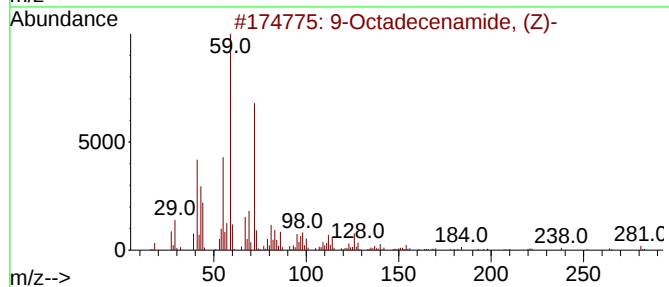
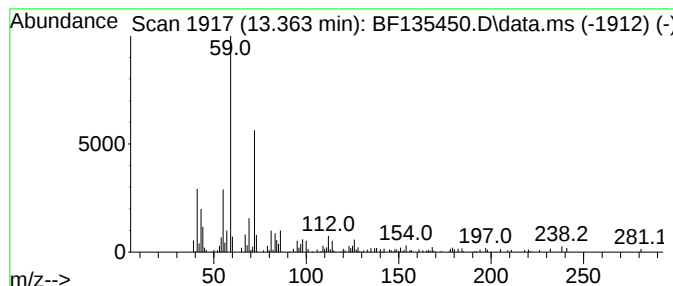
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.363	2.26 ng	91411	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	89
2			Hexadecanamide	255	C16H33NO	000629-54-9	72
3			Nonanamide	157	C9H19NO	001120-07-6	68
4			Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	53
5			Silane, hexyl-	116	C6H16Si	001072-14-6	50



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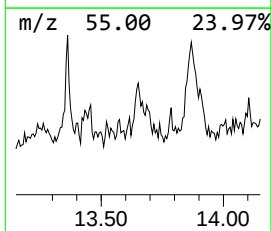
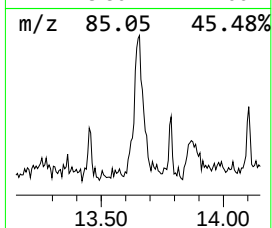
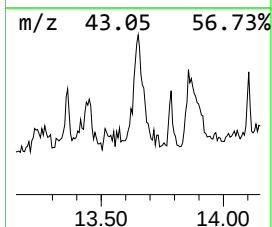
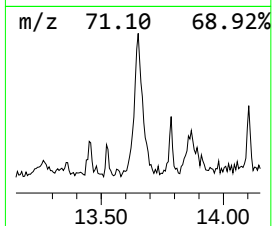
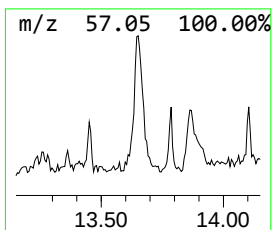
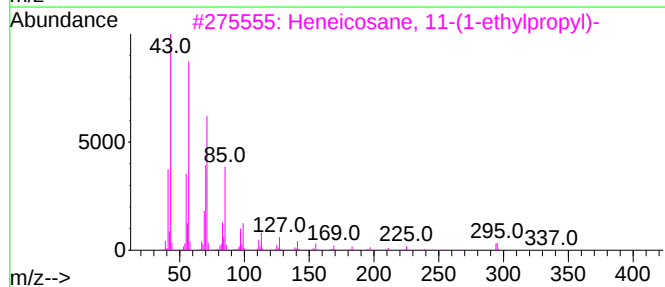
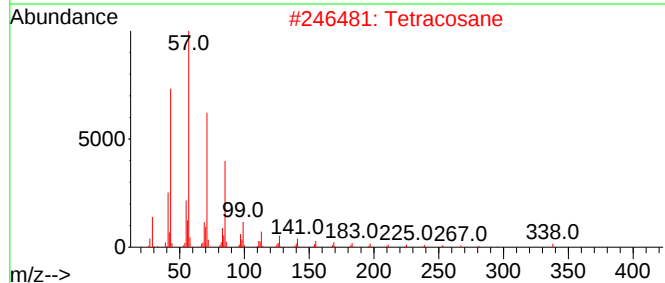
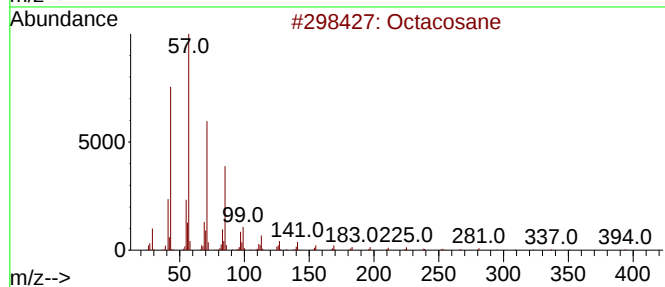
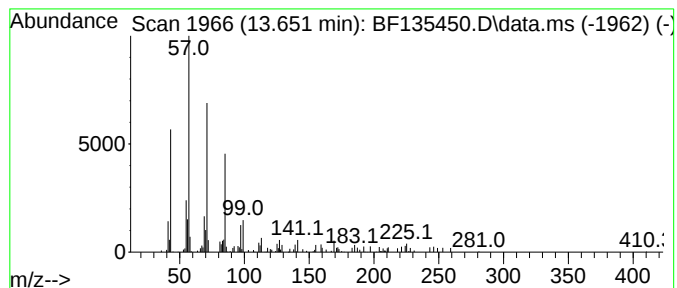
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.651	2.11 ng	85355	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Tetracosane	338	C24H50	000646-31-1	87
3			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
4			Hexacosane	366	C26H54	000630-01-3	83
5			Eicosane, 9-octyl-	394	C28H58	013475-77-9	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092623\
Data File : BF135450.D
Acq On : 26 Sep 2023 13:50
Operator : CG\JU
Sample : 04566-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

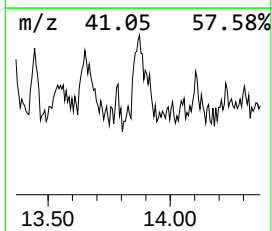
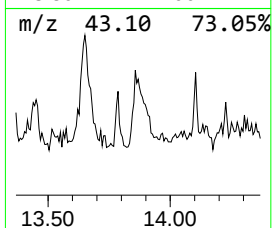
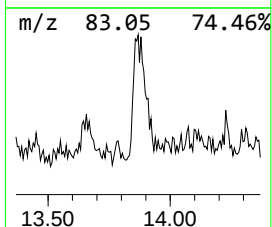
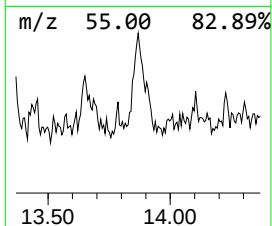
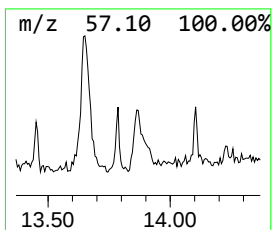
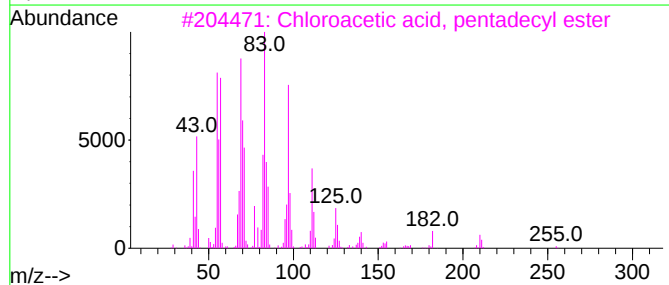
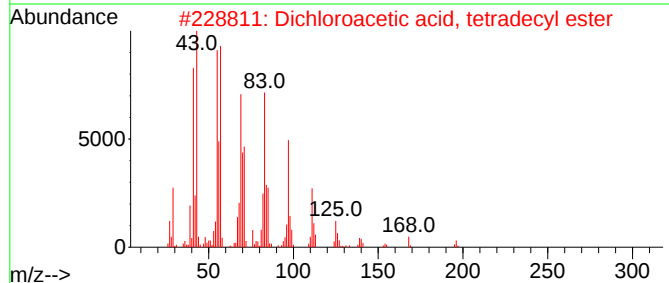
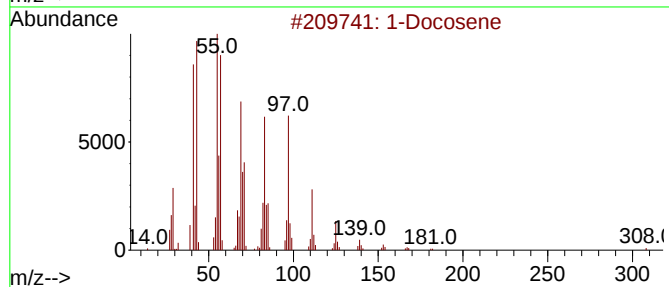
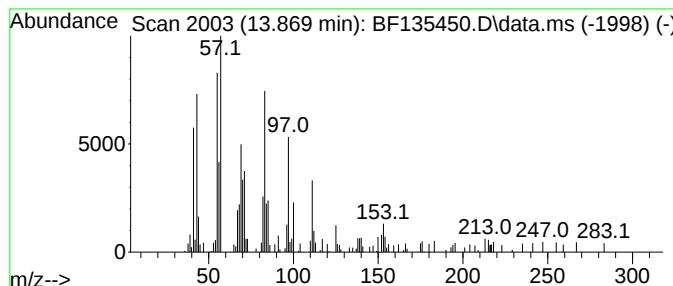
Instrument :
BNA_F
ClientSampleId :
CPT102-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.869	2.78 ng	112393	Chrysene-d12	13.939	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	87
3	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	87
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	87
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092623\
Data File : BF135450.D
Acq On : 26 Sep 2023 13:50
Operator : CG\JU
Sample : 04566-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CPT102-06

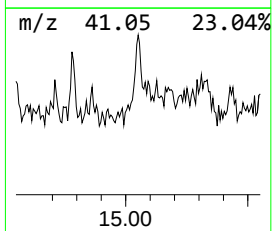
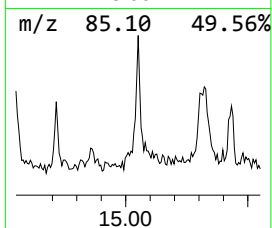
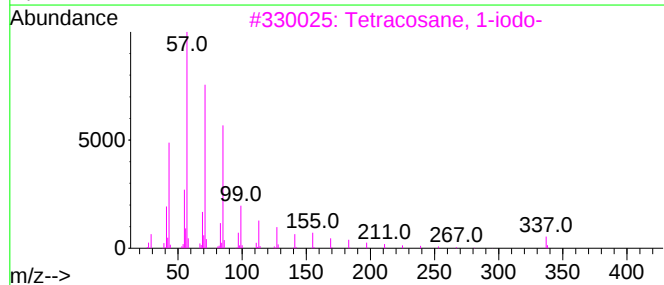
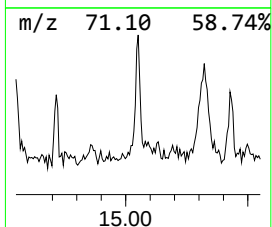
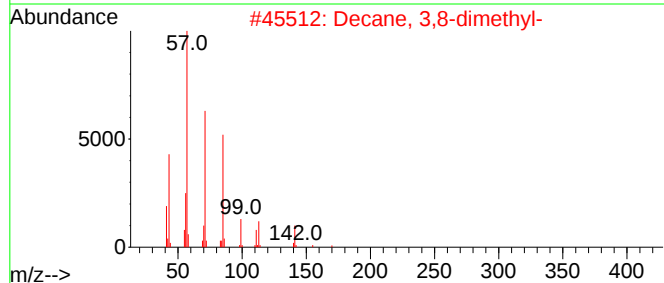
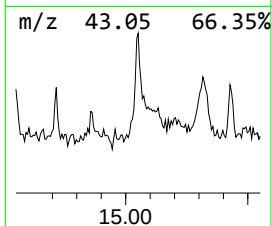
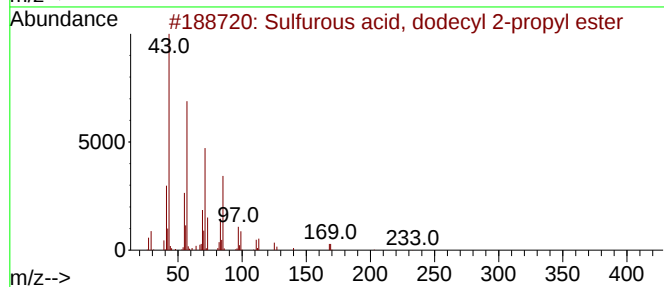
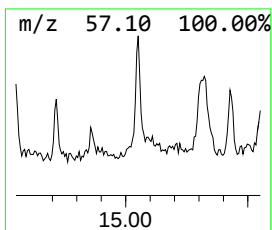
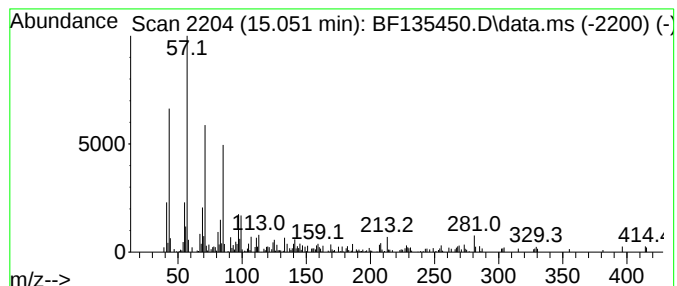
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Sulfurous acid, dodecyl 2-p... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.051	3.00 ng	153825	Perylene-d12	15.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	64
2			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	62
3			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	59
4			Octadecane	254	C18H38	000593-45-3	58
5			Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092623\
Data File : BF135450.D
Acq On : 26 Sep 2023 13:50
Operator : CG\JU
Sample : 04566-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CPT102-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-e...	6.604	2.2	ng	104549	1	6.751	963315	20.0
2,4,7,9-Tetrame...	9.234	10.3	ng	675515	3	9.786	1316690	20.0
n-Hexadecanoic ...	11.816	11.3	ng	726606	4	11.281	1282780	20.0
Octadecanoic acid	12.604	4.6	ng	293067	4	11.281	1282780	20.0
9-Octadecenamid...	13.363	2.3	ng	91411	5	13.939	809890	20.0
Octacosane	13.651	2.1	ng	85355	5	13.939	809890	20.0
1-Docosene	13.869	2.8	ng	112393	5	13.939	809890	20.0
Sulfurous acid,...	15.051	3.0	ng	153825	6	15.404	1026760	20.0