

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031324\
 Data File : BF137574.D
 Acq On : 13 Mar 2024 13:42
 Operator : CG\JU
 Sample : P1725-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-3860

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137574.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.251	22	28	36	rVB	1075847	1464917	4.55%	1.991%
2	5.581	589	594	597	rBV	4485525	4247216	13.18%	5.773%
3	6.551	755	759	785	rBV	4053785	4776362	14.83%	6.492%
4	6.910	816	820	831	rBV	1483417	1289041	4.00%	1.752%
5	7.463	910	914	926	rBV	2802783	2973189	9.23%	4.041%
6	8.175	1031	1035	1040	rBV	1740022	1719947	5.34%	2.338%
7	9.257	1214	1219	1222	rBV	5575489	5069631	15.74%	6.891%
8	9.933	1330	1334	1338	rBV	2380865	2056200	6.38%	2.795%
9	10.733	1465	1470	1473	rBV	3342161	3214782	9.98%	4.370%
10	11.433	1585	1589	1591	rBV	2376121	2088762	6.48%	2.839%
11	11.980	1677	1682	1691	rBV2	862778	1076824	3.34%	1.464%
12	12.651	1793	1796	1801	rBV	735027	671205	2.08%	0.912%
13	12.768	1811	1816	1828	rBV2	274690	469598	1.46%	0.638%
14	12.880	1830	1835	1839	rVV	592527	787892	2.45%	1.071%
15	13.039	1857	1862	1865	rBV	5171995	4793017	14.88%	6.515%
16	13.351	1896	1915	1929	rBV	9380999	32215312	100.00%	43.787%
17	13.951	2013	2017	2025	rBV3	438964	563470	1.75%	0.766%
18	14.098	2034	2042	2044	rBV2	1559802	1798121	5.58%	2.444%
19	15.180	2222	2226	2230	rBV	225556	360227	1.12%	0.490%
20	15.651	2301	2306	2315	rVV	1027210	1521949	4.72%	2.069%
21	18.350	2757	2765	2776	rBV5	129804	415318	1.29%	0.564%

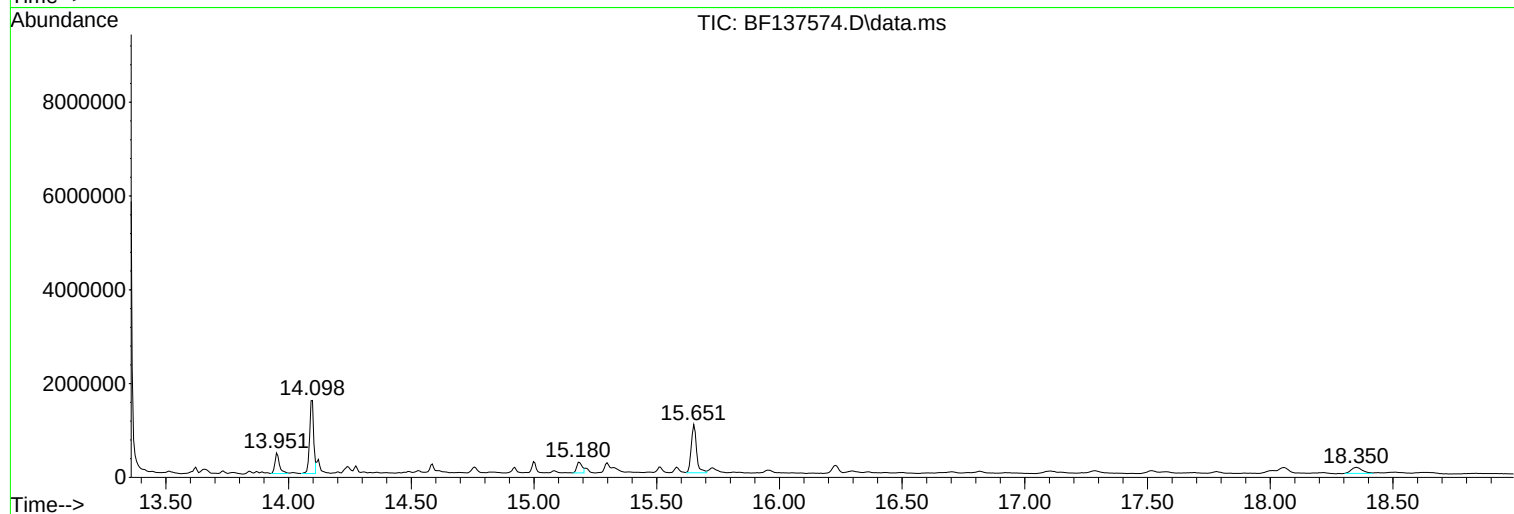
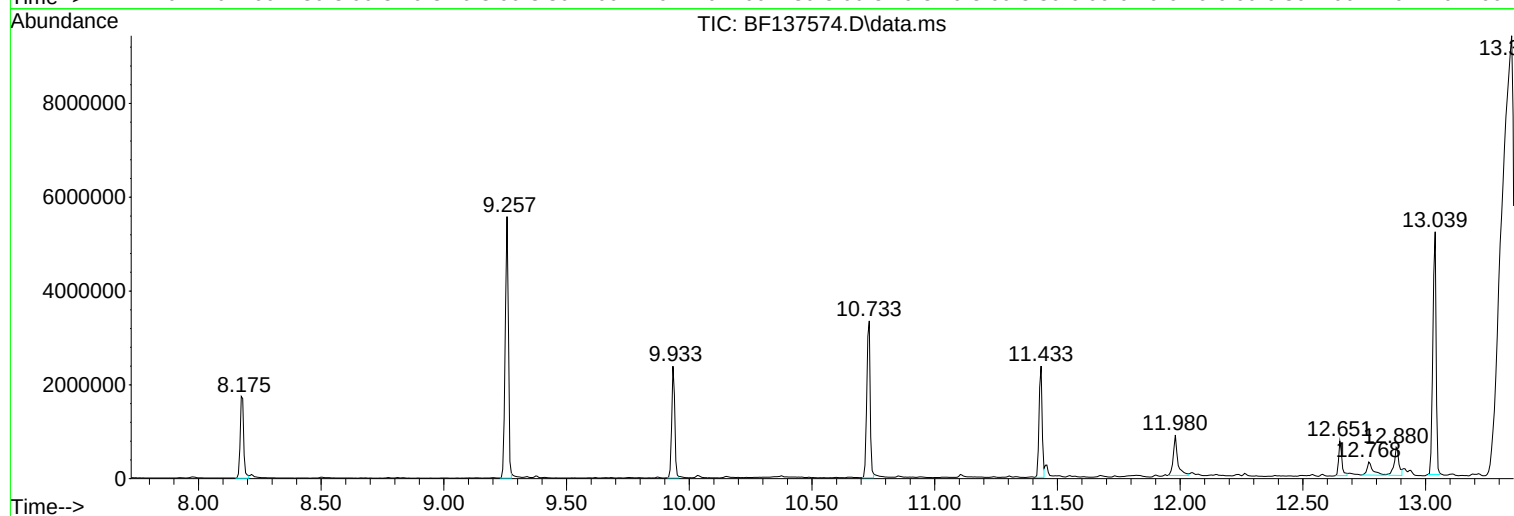
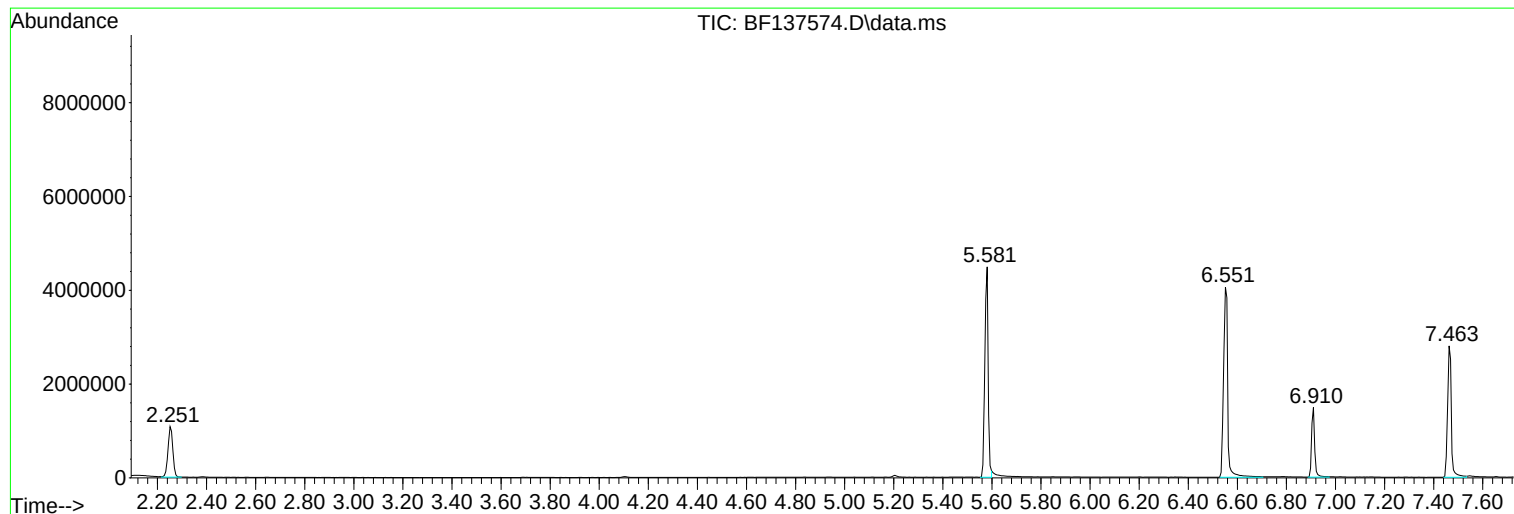
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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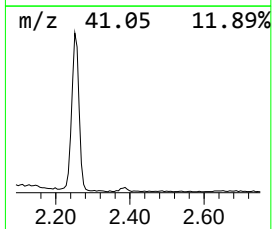
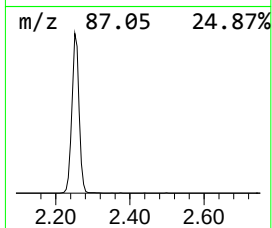
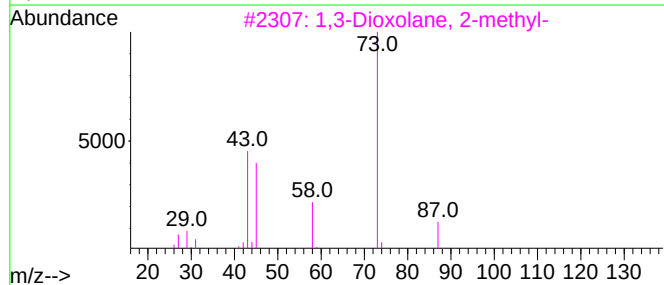
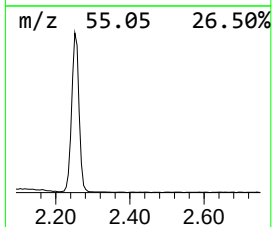
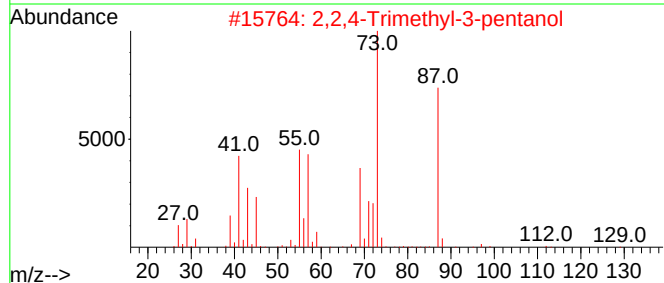
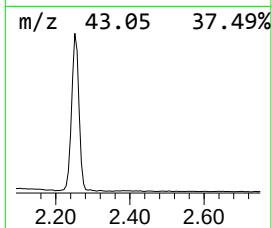
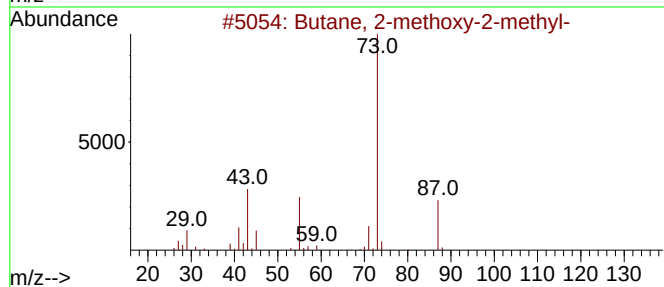
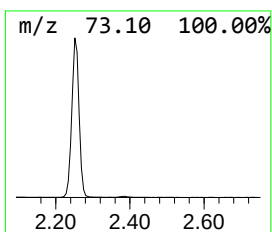
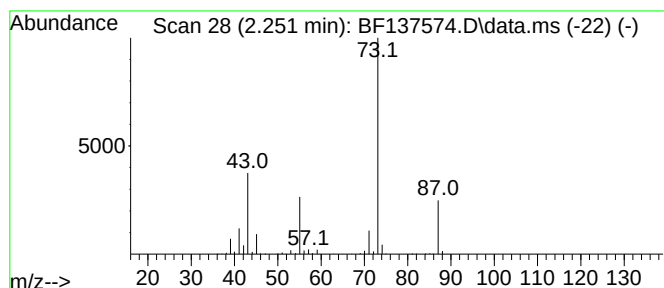
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.251	22.73 ng	1464920	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17



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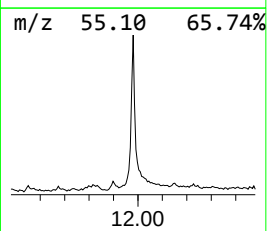
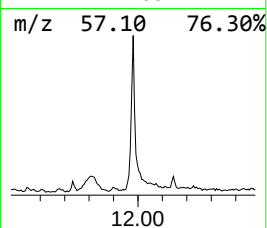
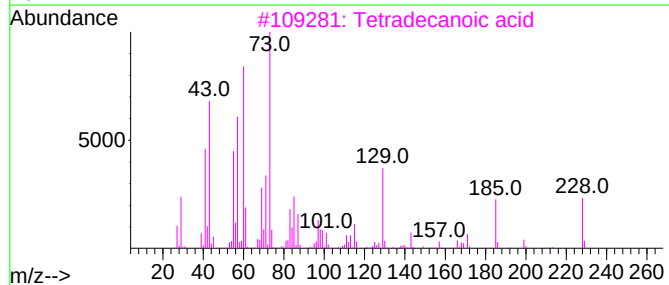
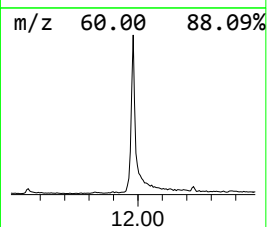
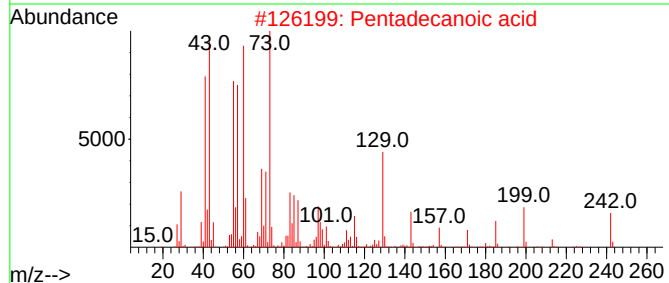
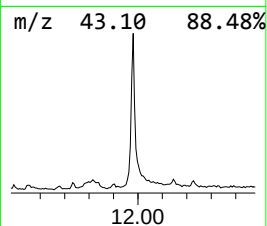
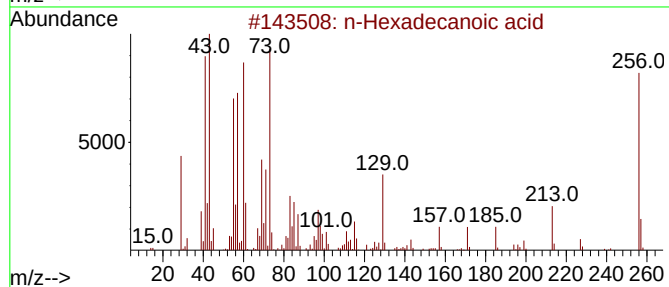
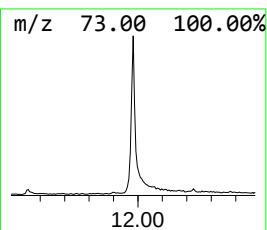
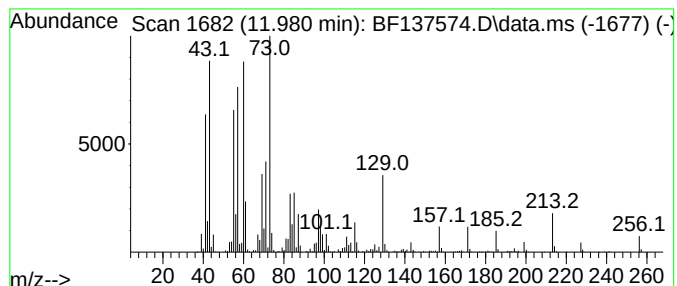
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.980	10.31 ng	1076820	Phenanthrene-d10		11.433
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	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	53



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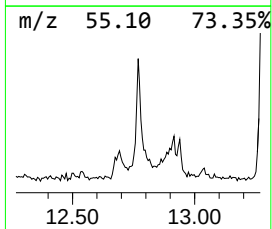
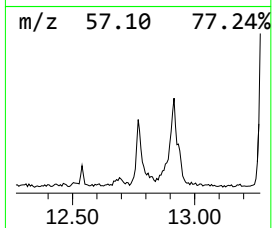
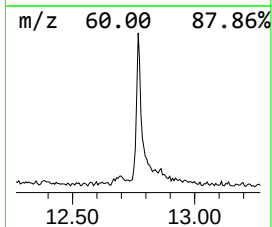
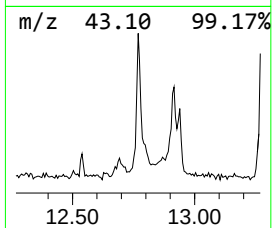
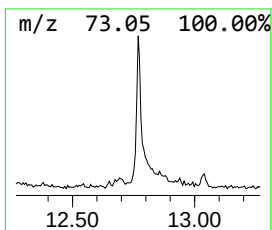
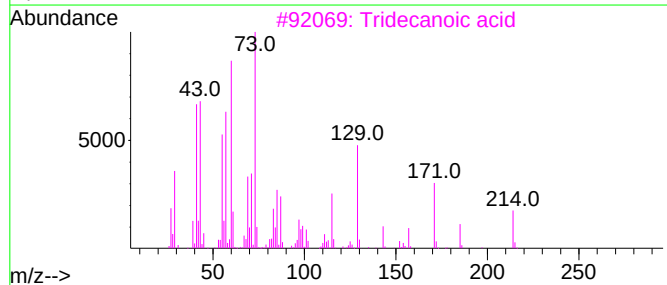
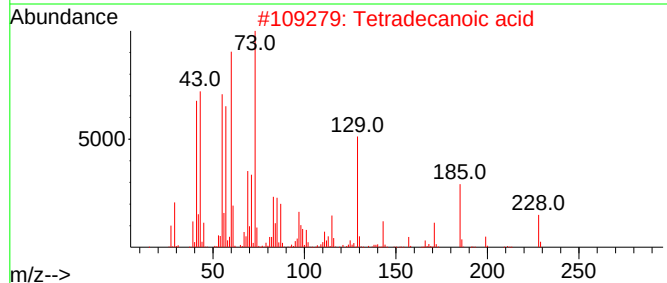
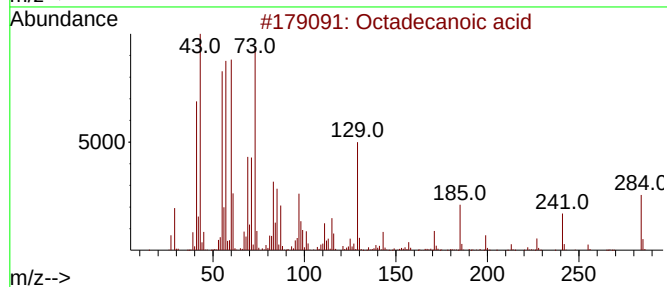
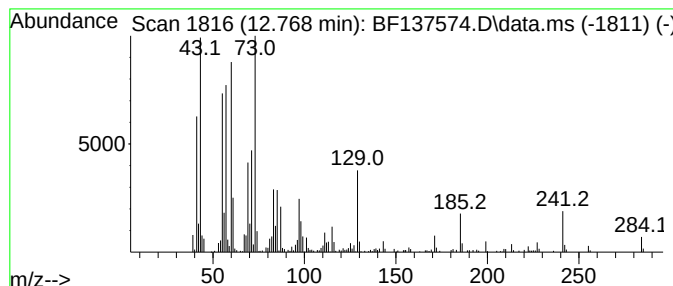
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.768	5.22 ng	469598	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	30



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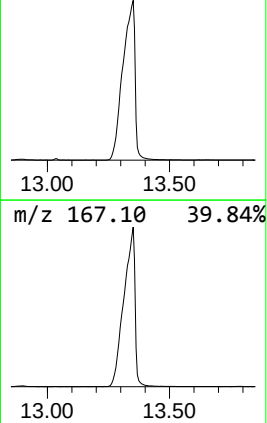
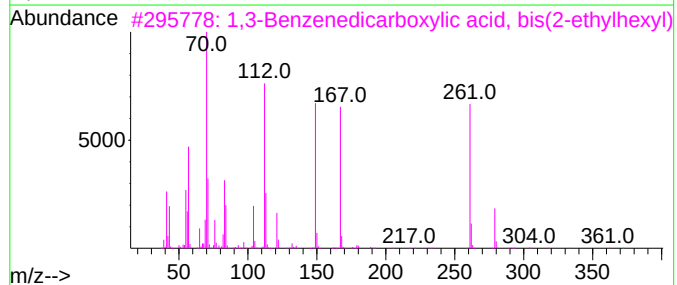
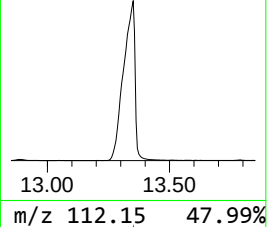
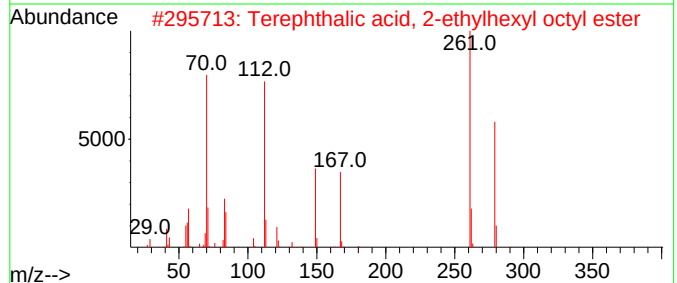
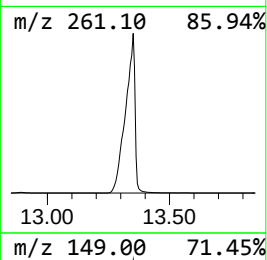
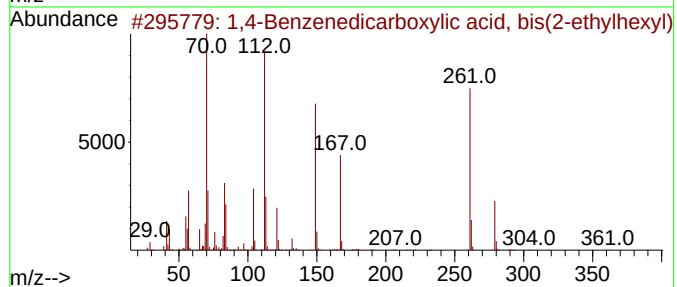
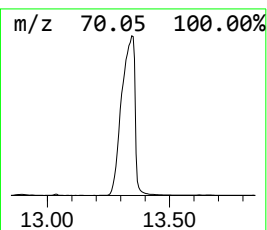
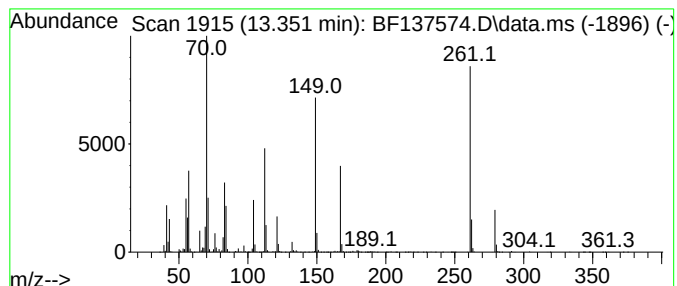
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,4-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.351	358.32 ng	32215300	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	87
2			Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	68
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	64
4			Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	62
5			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	50



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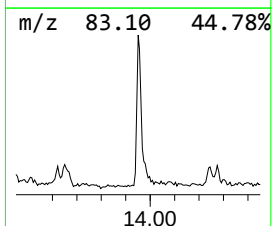
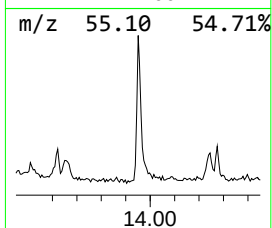
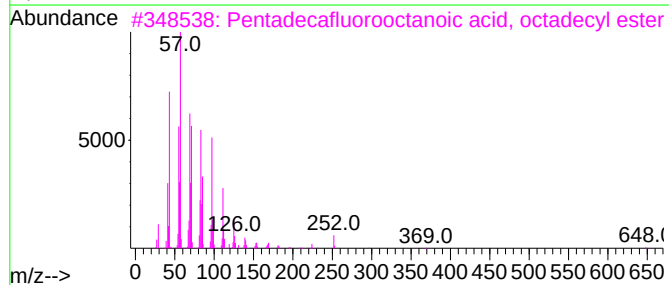
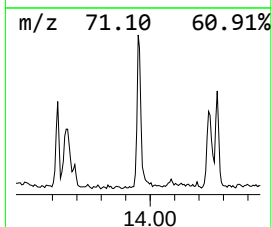
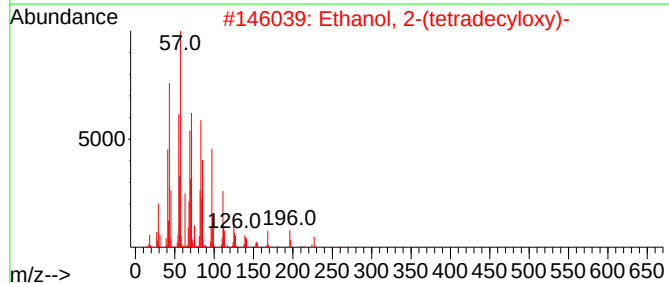
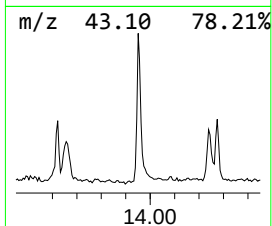
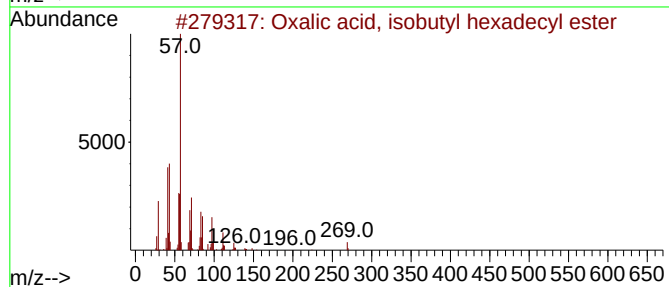
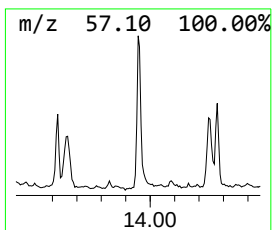
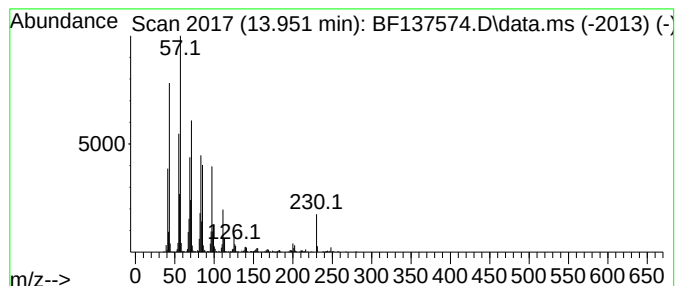
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Peak Number 5 Oxalic acid, isobutyl hexadec... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.951	6.27 ng	563470	Chrysene-d12	14.098	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	83
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	70
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	70



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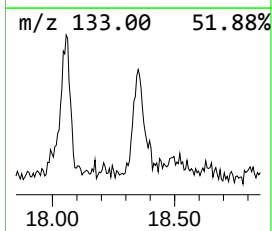
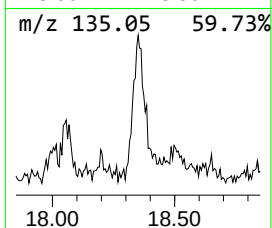
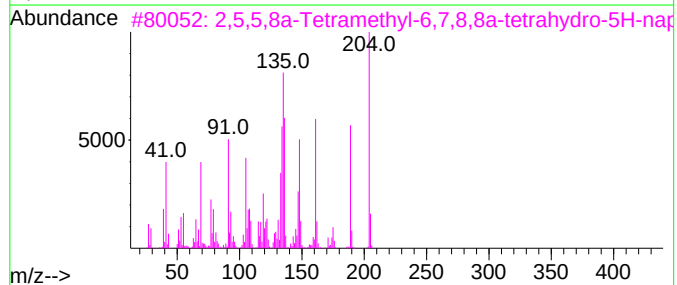
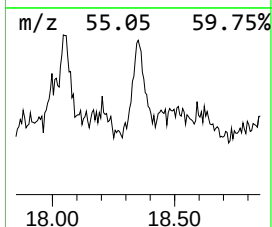
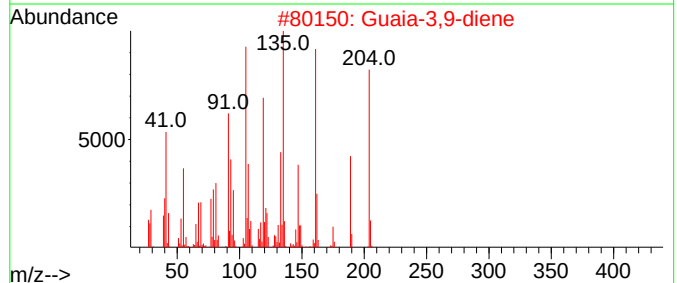
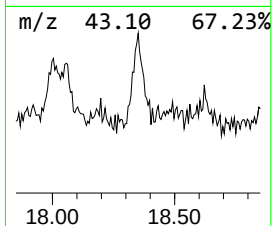
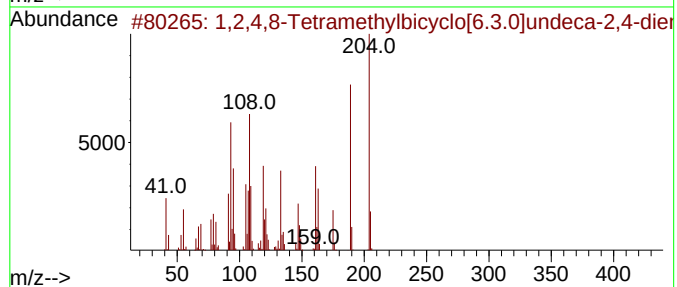
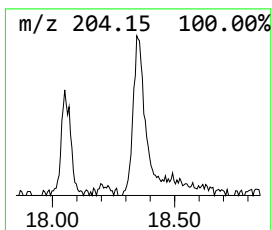
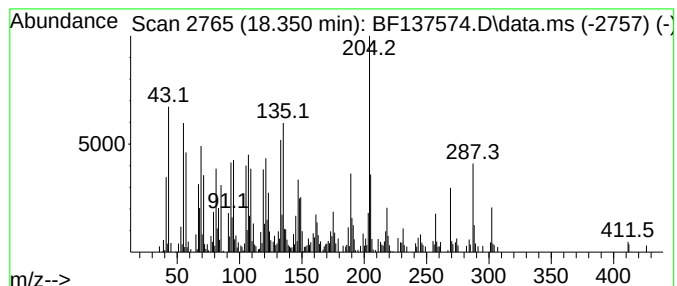
Instrument :
BNA_F
ClientSampleId :
RT-3860

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,2,4,8-Tetramethylbicyclo[... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.350	5.46 ng	415318	Perylene-d12	15.651	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,8-Tetramethylbicyclo[6.3.0...]	204	C15H24	137235-51-9	53
2	Guaia-3,9-diene	204	C15H24	000489-83-8	46
3	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	46
4	1-(4-Amino-2-methylphenyl)-2-pip...	204	C12H16N2O	443999-53-9	45
5	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031324\
Data File : BF137574.D
Acq On : 13 Mar 2024 13:42
Operator : CG\JU
Sample : P1725-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-3860

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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
Butane, 2-metho...	2.251	22.7	ng	1464920	1	6.910	1289040	20.0
n-Hexadecanoic ...	11.980	10.3	ng	1076820	4	11.433	2088760	20.0
Octadecanoic acid	12.768	5.2	ng	469598	5	14.098	1798120	20.0
1,4-Benzenedica...	13.351	358.3	ng	32215300	5	14.098	1798120	20.0
Oxalic acid, is...	13.951	6.3	ng	563470	5	14.098	1798120	20.0
1,2,4,8-Tetrame...	18.350	5.5	ng	415318	6	15.651	1521950	20.0