

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091823\
 Data File : BF135319.D
 Acq On : 18 Sep 2023 21:51
 Operator : CG\JU
 Sample : 04441-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11976

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: BF135319.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	494	498	509	rVB	79715	126445	3.02%	0.479%
2	5.398	558	563	566	rBV	3777291	3983774	95.28%	15.106%
3	6.404	728	734	737	rBV	3455505	4069004	97.32%	15.429%
4	6.757	790	794	797	rBV	917687	763101	18.25%	2.894%
5	7.322	885	890	893	rBV	2504321	2699792	64.57%	10.237%
6	8.034	1007	1011	1016	rBV	1092359	951631	22.76%	3.608%
7	9.116	1189	1195	1198	rBV	4247510	4180928	100.00%	15.854%
8	9.233	1210	1215	1227	rVB	44849	55474	1.33%	0.210%
9	9.792	1305	1310	1313	rBV	1107905	971634	23.24%	3.684%
10	10.586	1440	1445	1448	rBV	2313571	2192385	52.44%	8.313%
11	11.280	1560	1563	1566	rBV	984377	856005	20.47%	3.246%
12	11.304	1566	1567	1571	rVV	150618	100485	2.40%	0.381%
13	11.357	1571	1576	1580	rVB	41320	45985	1.10%	0.174%
14	11.822	1651	1655	1665	rBV	326526	348551	8.34%	1.322%
15	12.504	1766	1771	1775	rBV	180689	170041	4.07%	0.645%
16	12.610	1785	1789	1794	rBV	67262	84732	2.03%	0.321%
17	12.733	1804	1810	1813	rBV	137754	144394	3.45%	0.548%
18	12.880	1831	1835	1838	rBV	2626297	2452825	58.67%	9.301%
19	13.833	1992	1997	2007	rVB8	48641	134215	3.21%	0.509%
20	13.939	2010	2015	2018	rVV	663802	662026	15.83%	2.510%
21	13.963	2018	2019	2022	rVB	97587	63068	1.51%	0.239%
22	14.533	2108	2116	2120	rBV4	41767	100956	2.41%	0.383%
23	14.574	2120	2123	2128	rBV	211853	232661	5.56%	0.882%
24	14.980	2188	2192	2195	rBV	78249	107475	2.57%	0.408%
25	15.280	2239	2243	2247	rVB	45547	57284	1.37%	0.217%
26	15.339	2250	2253	2259	rVB	49846	67313	1.61%	0.255%
27	15.404	2259	2264	2269	rBV	561513	705310	16.87%	2.674%
28	15.880	2341	2345	2351	rVB2	26493	44753	1.07%	0.170%

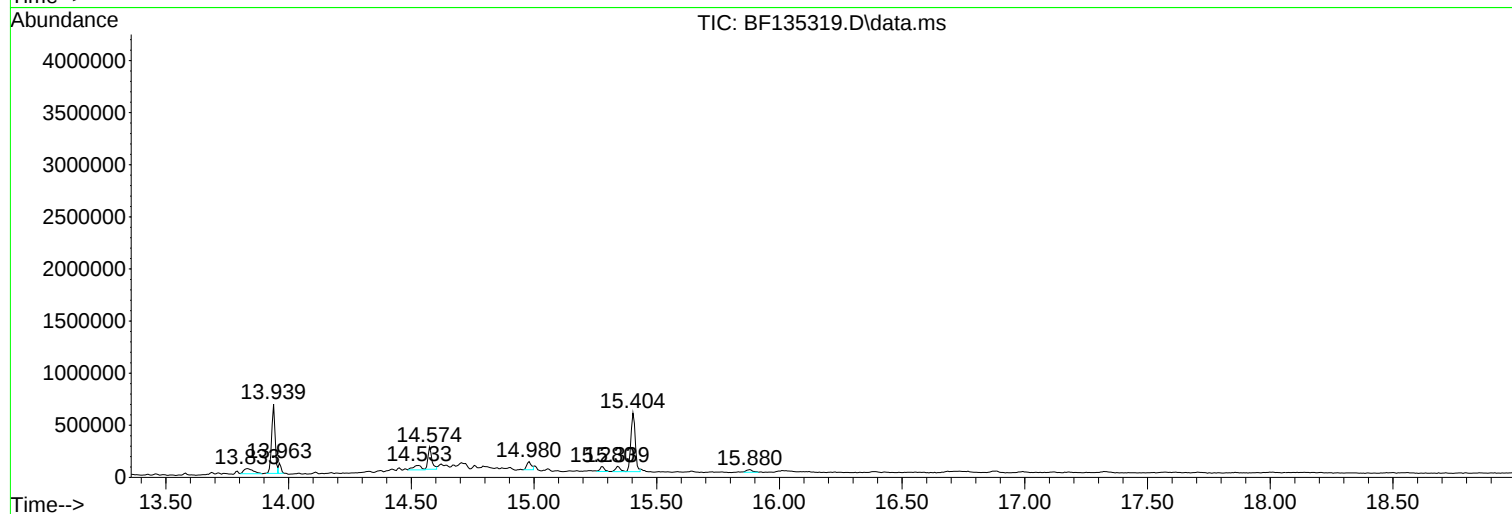
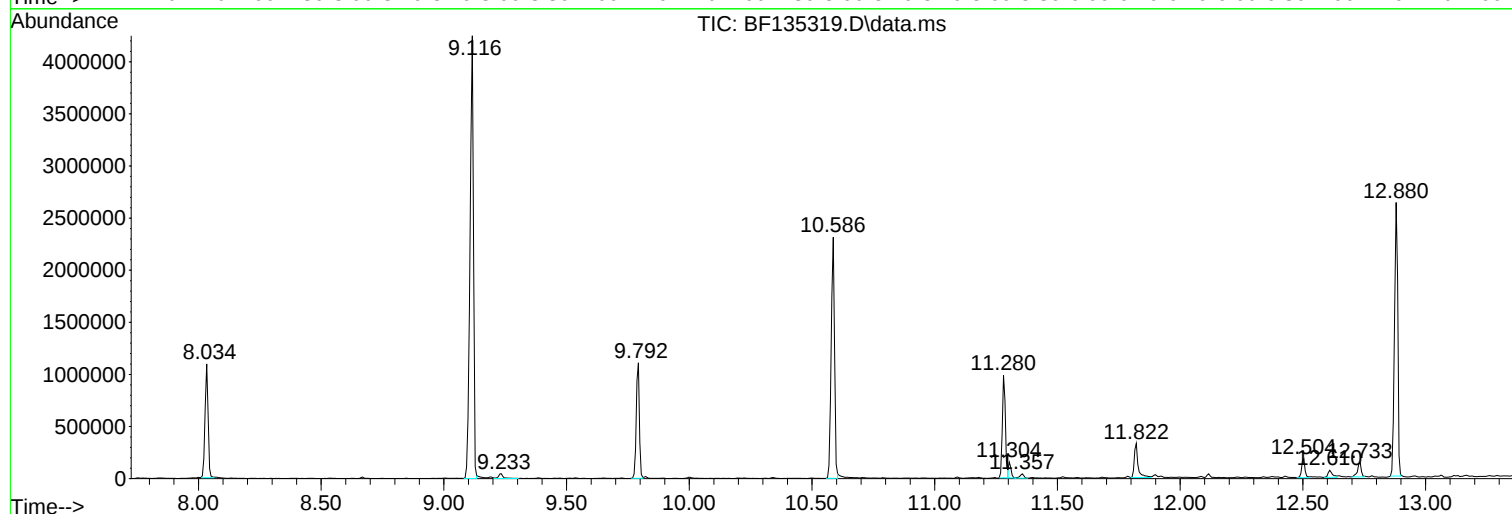
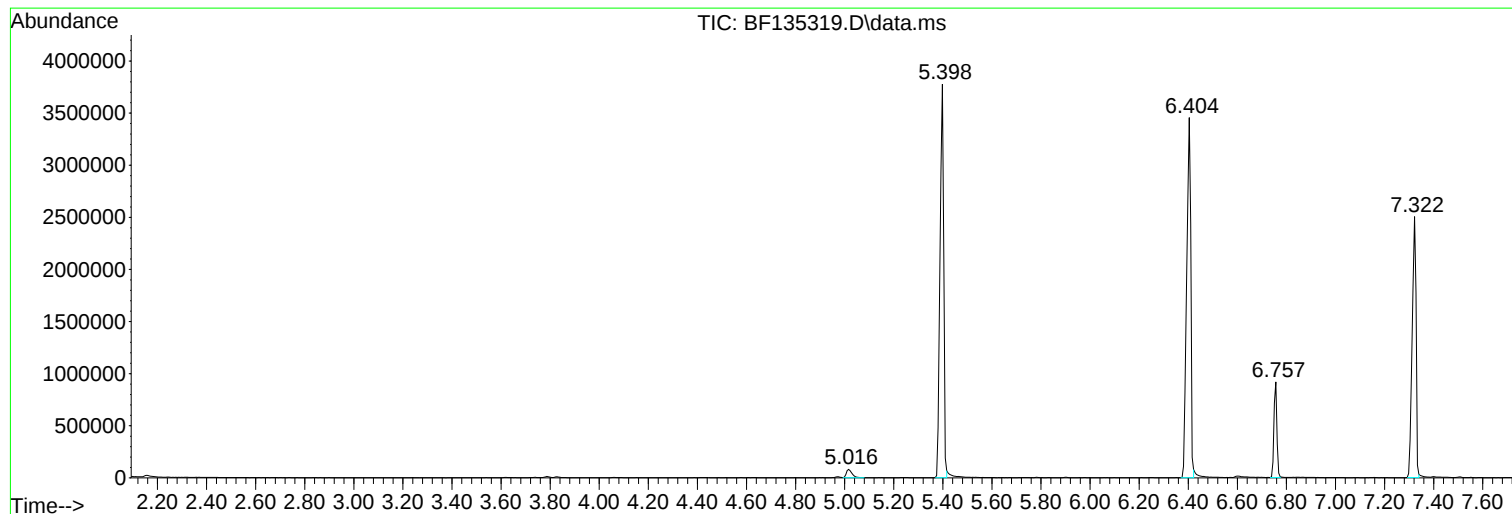
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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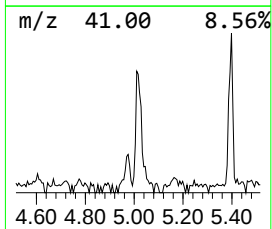
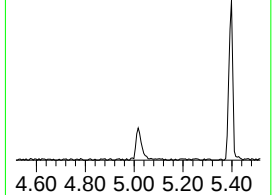
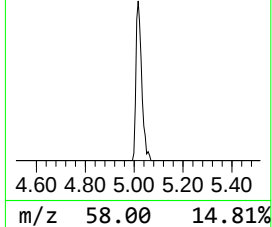
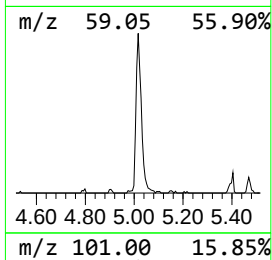
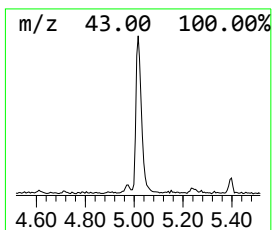
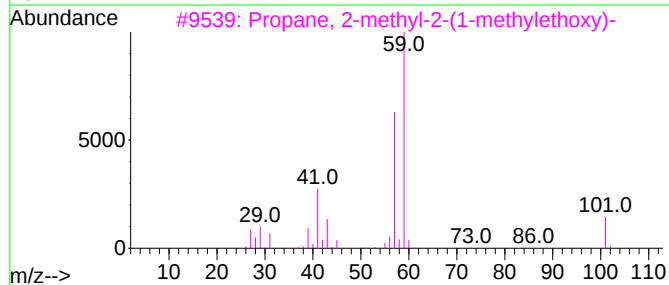
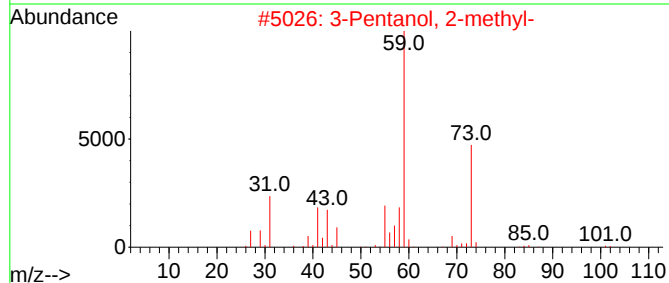
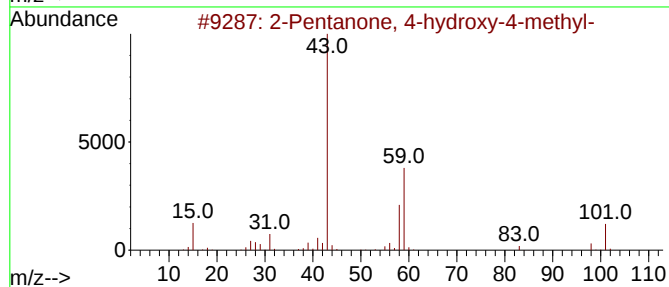
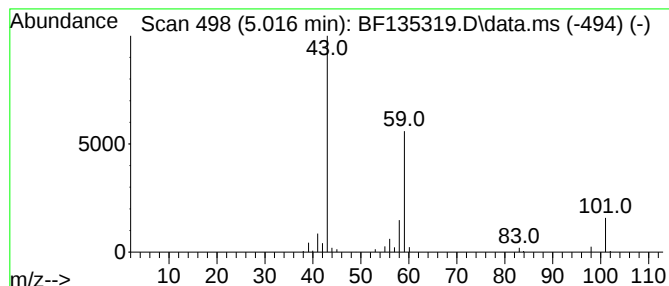
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	3.31 ng	126445	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	50		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25		



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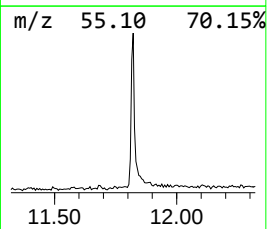
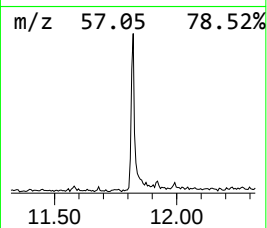
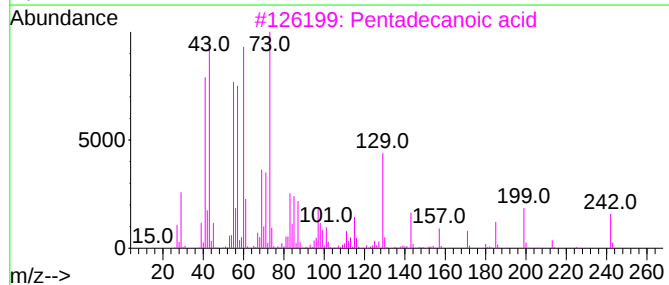
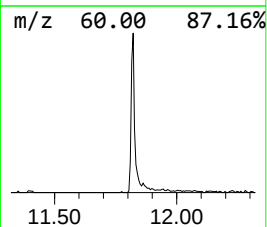
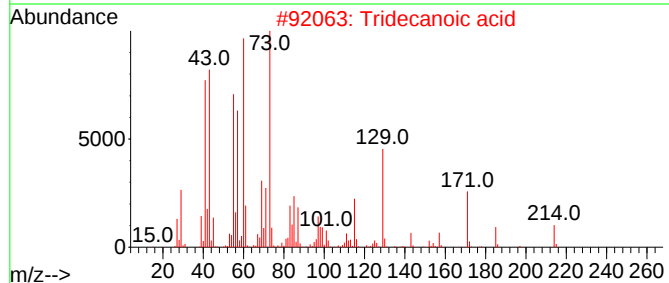
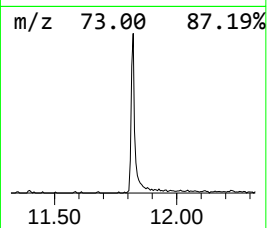
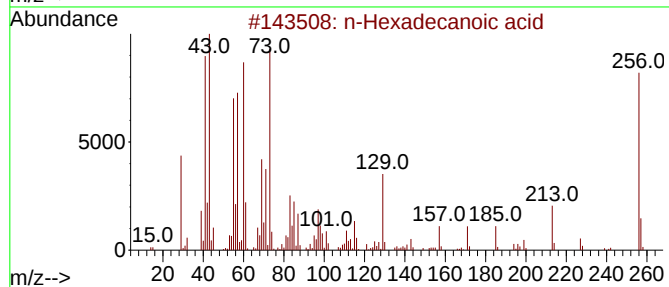
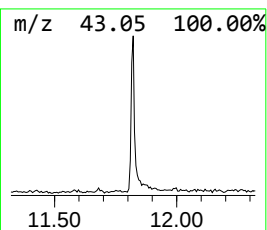
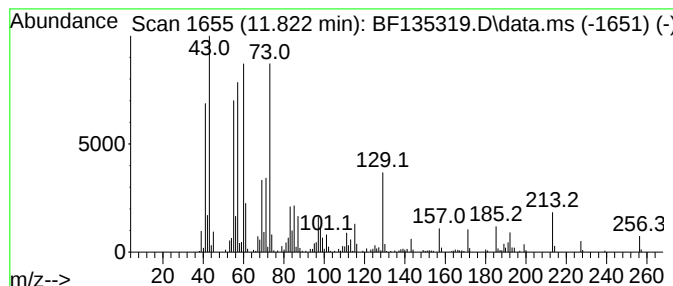
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	8.14 ng	348551	Phenanthrene-d10	11.280

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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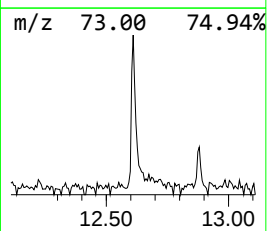
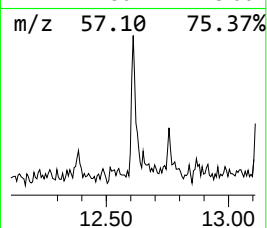
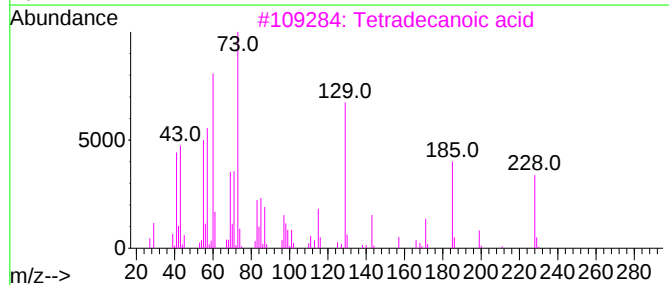
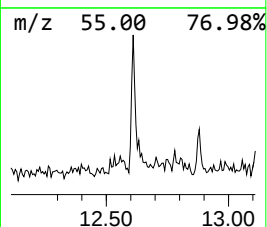
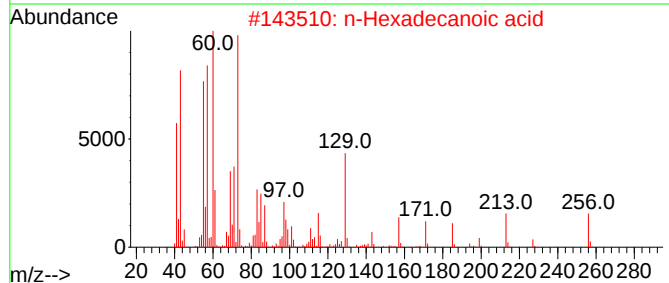
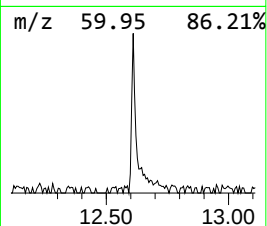
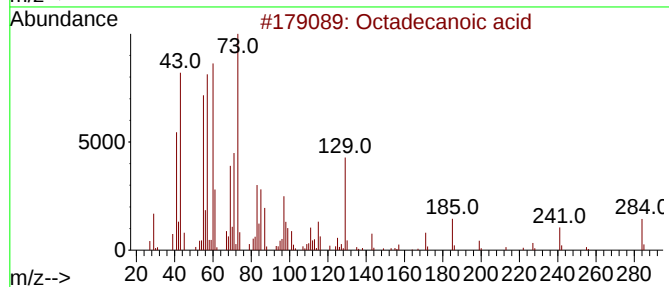
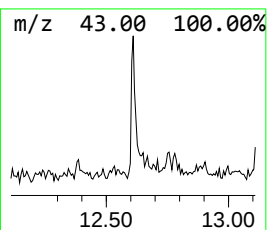
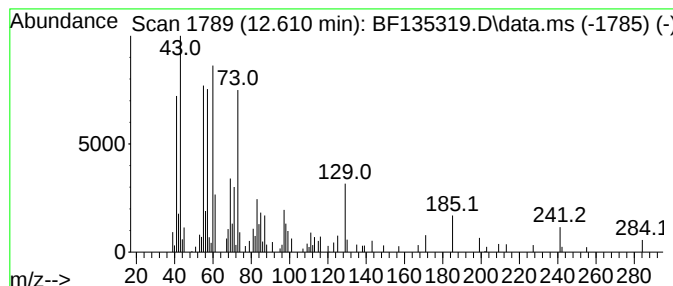
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Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	2.56 ng	84732	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	76
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	43
5			Tridecanoic acid	214	C13H26O2	000638-53-9	35



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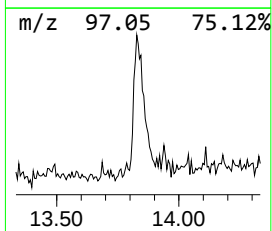
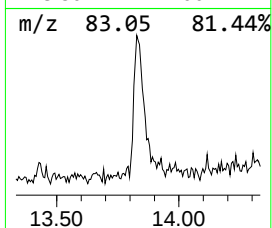
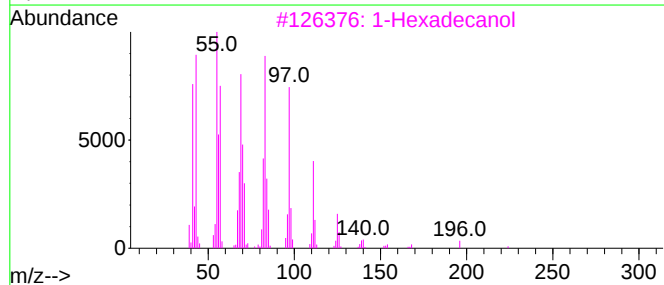
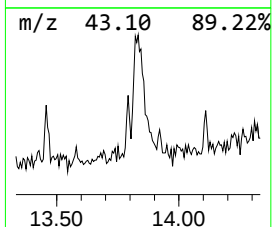
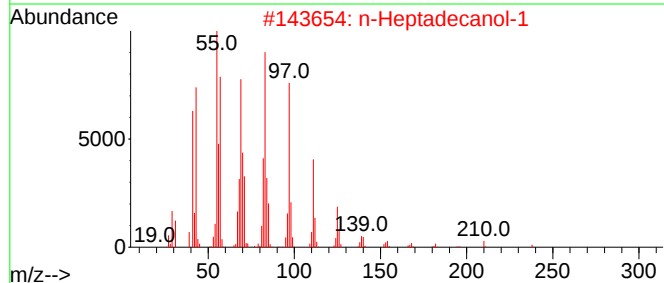
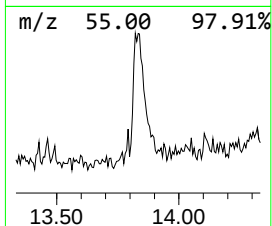
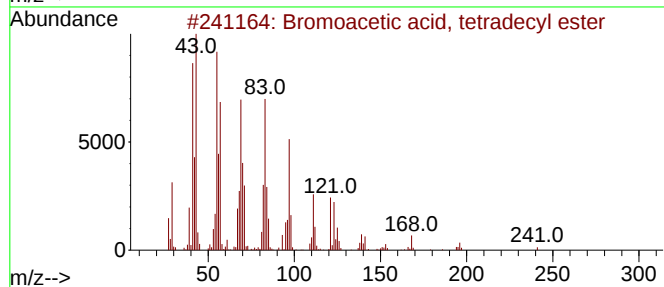
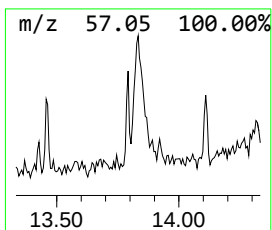
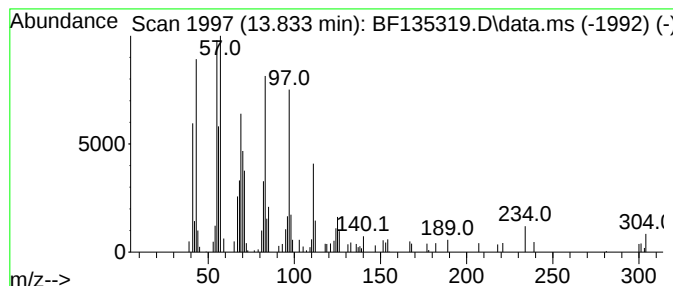
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Peak Number 4 Bromoacetic acid, tetradecyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	4.05 ng	134215	Chrysene-d12	13.939

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, tetradecyl ester	334	C16H31BrO2	018992-01-3	90
2		n-Heptadecanol-1	256	C17H36O	001454-85-9	90
3		1-Hexadecanol	242	C16H34O	036653-82-4	90
4		E-15-Heptadecenal	252	C17H32O	1000130-97-9	90
5		1-Octadecanol	270	C18H38O	000112-92-5	87



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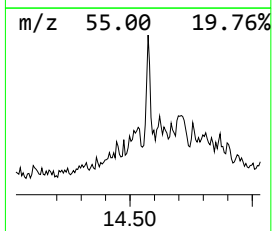
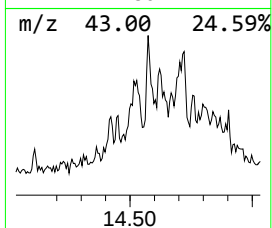
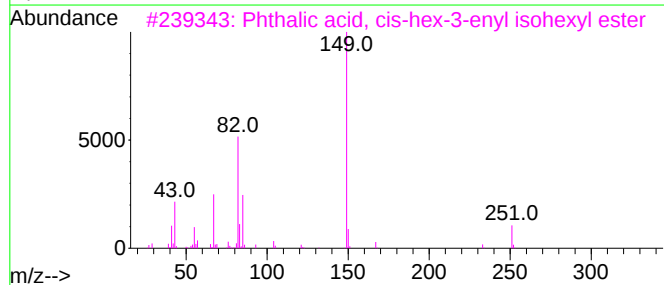
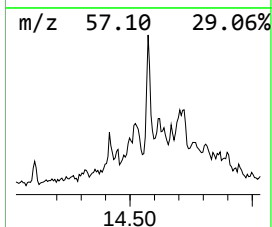
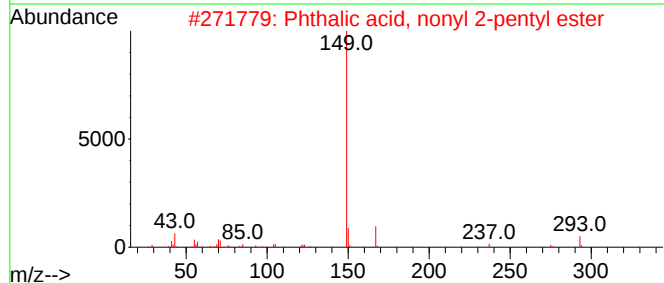
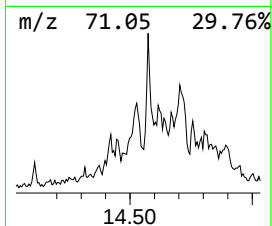
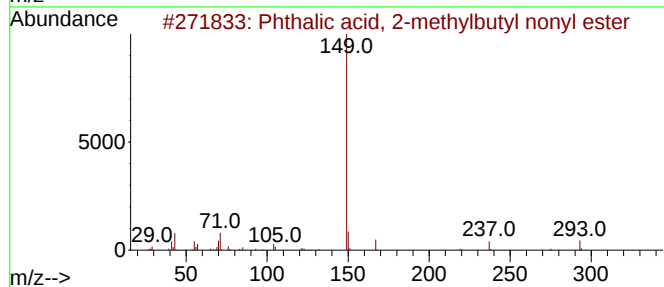
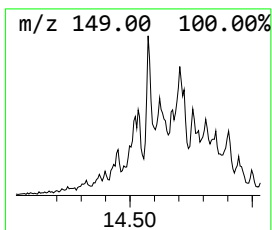
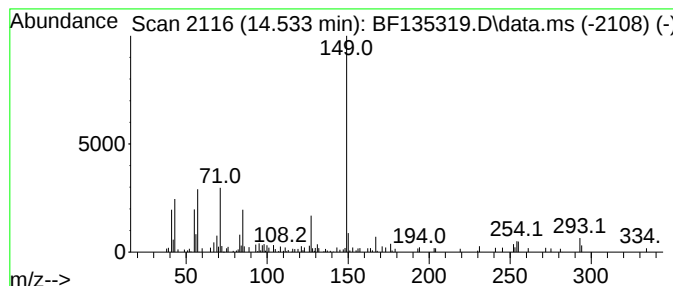
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Peak Number 5 Phthalic acid, 2-methylbuty... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	3.05 ng	100956	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, 2-methylbutyl non...	362	C22H34O4	1000322-81-7	53
2			Phthalic acid, nonyl 2-pentyl ester	362	C22H34O4	1000315-48-1	50
3			Phthalic acid, cis-hex-3-enyl is...	332	C20H28O4	1000360-36-7	50
4			Phthalic acid, hept-4-yl nonyl e...	390	C24H38O4	1000356-79-0	47
5			1,2-Benzenedicarboxylic acid, de...	418	C26H42O4	000119-07-3	47



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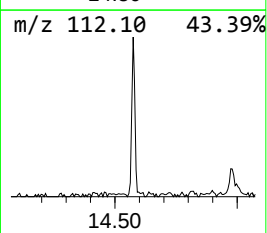
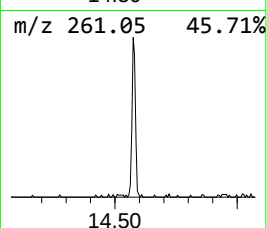
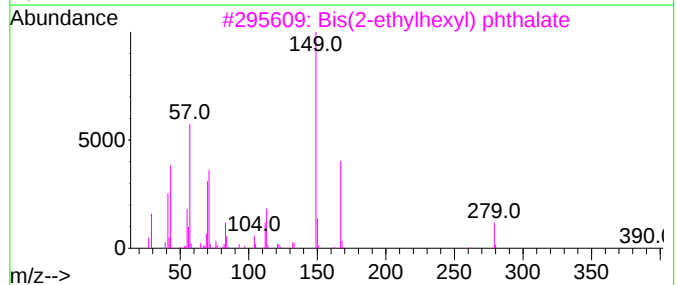
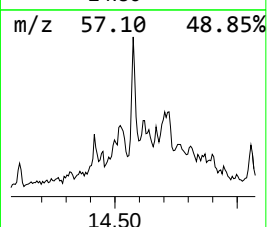
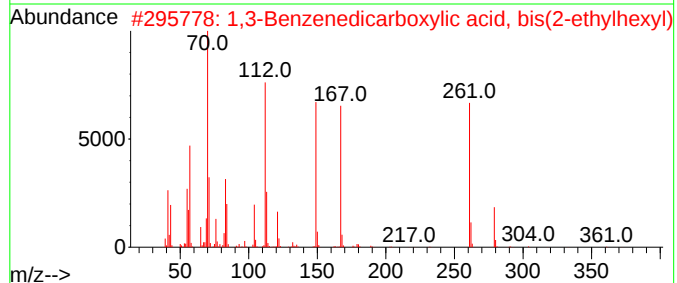
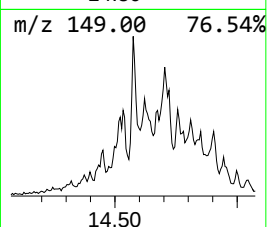
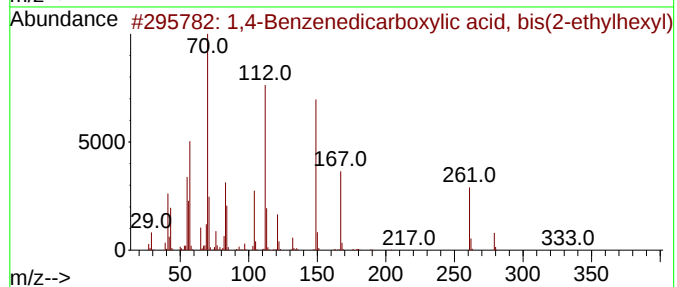
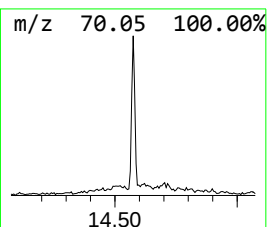
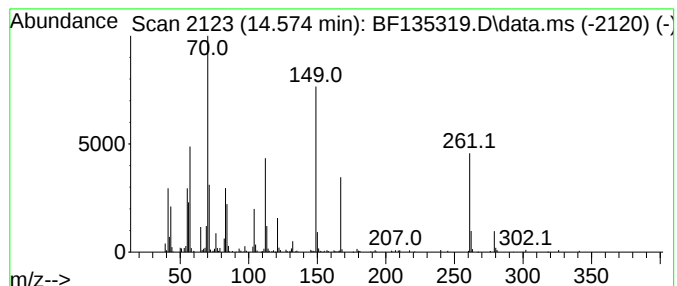
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.574	7.03 ng	232661	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	59
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	49
3			Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	38
4			2-((2-Ethylbutoxy)carbonyl)benzo...	250	C14H18O4	091401-46-6	27
5			Phthalic acid, octyl oct-3-yl ester	390	C24H38O4	1000377-71-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091823\
Data File : BF135319.D
Acq On : 18 Sep 2023 21:51
Operator : CG\JU
Sample : 04441-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11976

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
2-Pentanone, 4-...	5.016	3.3	ng	126445	1	6.757	763101	20.0
n-Hexadecanoic ...	11.822	8.1	ng	348551	4	11.280	856005	20.0
Octadecanoic acid	12.610	2.6	ng	84732	5	13.939	662026	20.0
Bromoacetic aci...	13.833	4.0	ng	134215	5	13.939	662026	20.0
Phthalic acid, ...	14.533	3.0	ng	100956	5	13.939	662026	20.0
1,4-Benzenedica...	14.574	7.0	ng	232661	5	13.939	662026	20.0