

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090421\
 Data File : BF125364.D
 Acq On : 4 Sep 2021 12:23
 Operator : JU/CG
 Sample : M3648-09
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20211058-SI-COMP-3-MODIFIED-EL

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-BF081821.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125364.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	13	23	31	rVB	3038055	4358444	100.00%	14.935%
2	5.122	512	516	523	rVB	51315	60085	1.38%	0.206%
3	5.522	580	584	599	rBV	2513484	2251157	51.65%	7.714%
4	6.522	750	754	766	rBV	1848891	1674677	38.42%	5.739%
5	6.898	814	818	821	rBV	1031701	836396	19.19%	2.866%
6	7.463	907	914	917	rBV	2559322	2551929	58.55%	8.745%
7	8.092	1016	1021	1032	rBV3	27983	75913	1.74%	0.260%
8	8.181	1032	1036	1043	rVV	1212932	1064901	24.43%	3.649%
9	9.257	1214	1219	1222	rBV	4730988	4210721	96.61%	14.429%
10	9.933	1330	1334	1338	rBV	1229056	1128916	25.90%	3.868%
11	10.727	1464	1469	1472	rBV	2942811	2555385	58.63%	8.757%
12	11.422	1583	1587	1594	rBV	1192740	1067843	24.50%	3.659%
13	11.580	1611	1614	1618	rBV	1372269	1124139	25.79%	3.852%
14	11.804	1649	1652	1655	rVB2	128489	95949	2.20%	0.329%
15	11.939	1671	1675	1679	rBV	313195	303302	6.96%	1.039%
16	11.980	1679	1682	1689	rVB	51679	69411	1.59%	0.238%
17	12.727	1803	1809	1816	rBV	83663	110891	2.54%	0.380%
18	13.010	1852	1857	1860	rBV	4294198	3696453	84.81%	12.667%
19	13.892	2003	2007	2010	rBV2	41424	48193	1.11%	0.165%
20	13.927	2010	2013	2016	rBV	118797	163335	3.75%	0.560%
21	14.063	2033	2036	2041	rVB	900836	766559	17.59%	2.627%
22	14.821	2161	2165	2171	rBV3	69189	100129	2.30%	0.343%
23	15.557	2285	2290	2302	rVB2	637117	867904	19.91%	2.974%

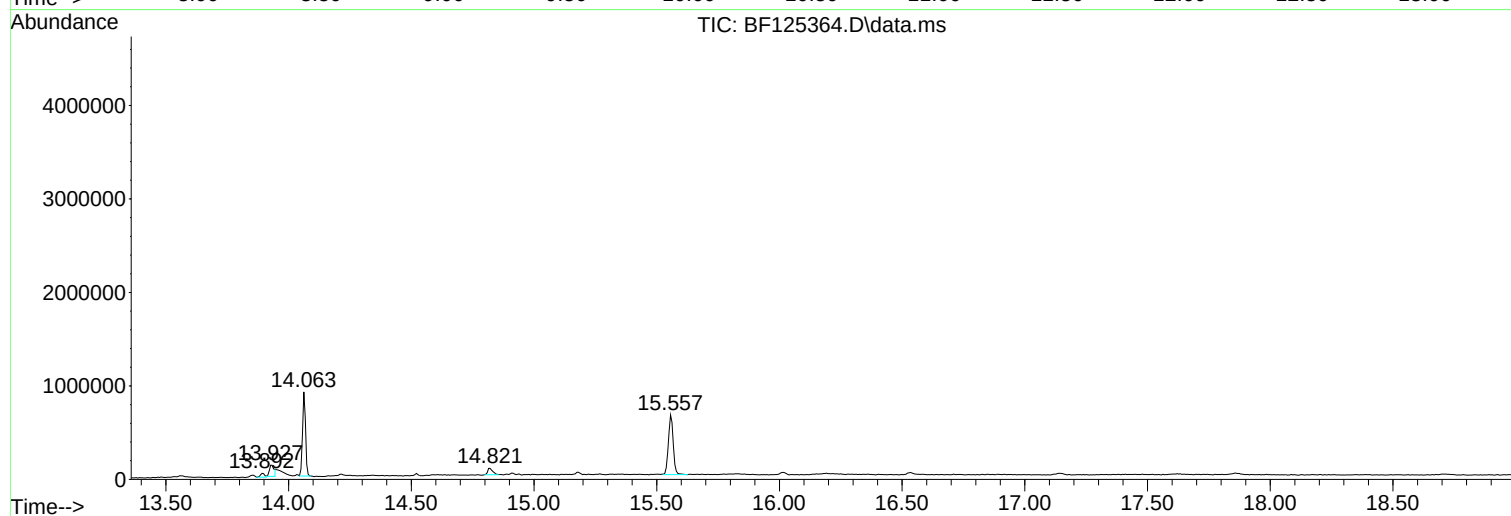
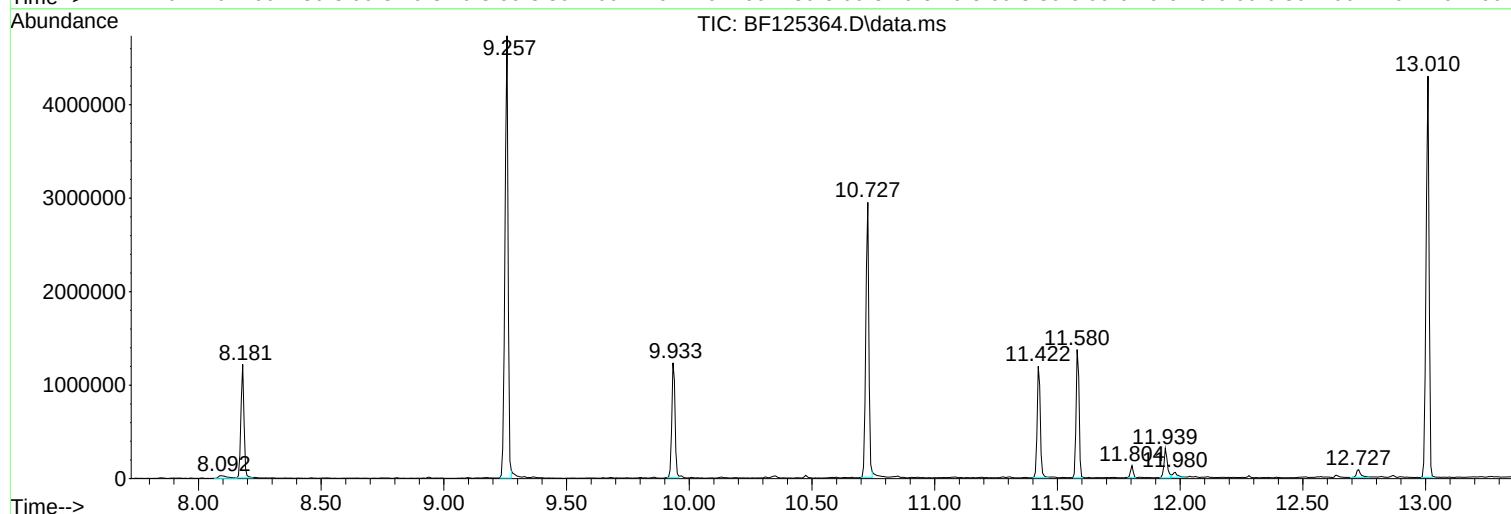
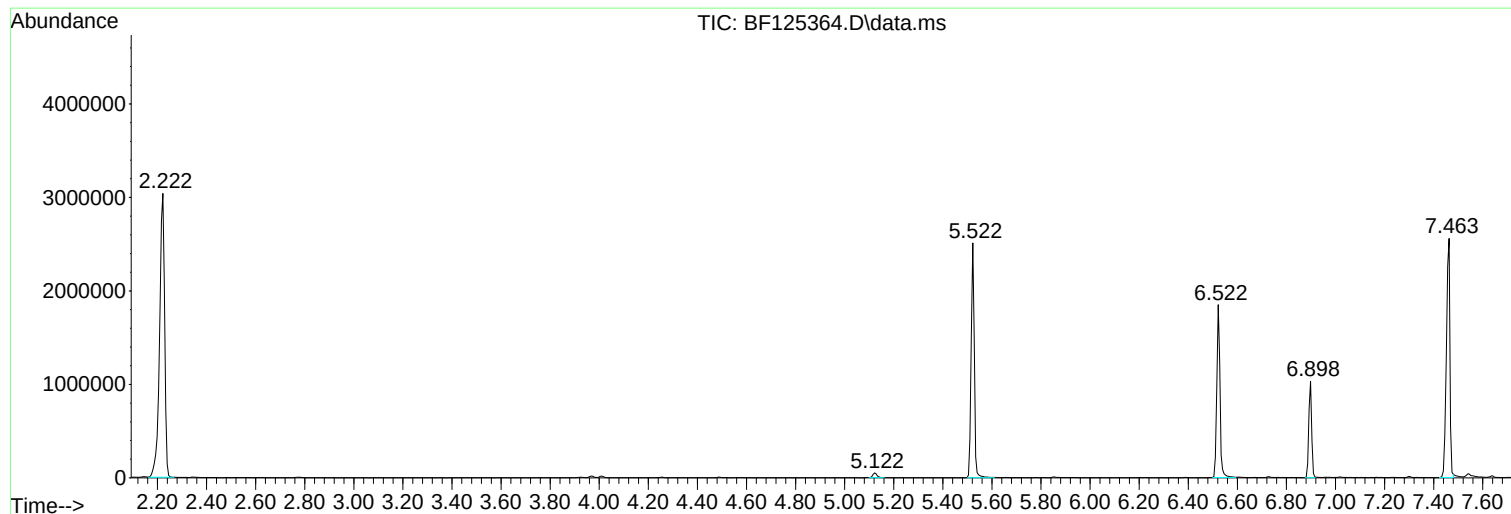
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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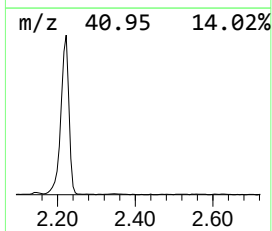
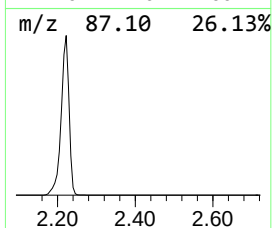
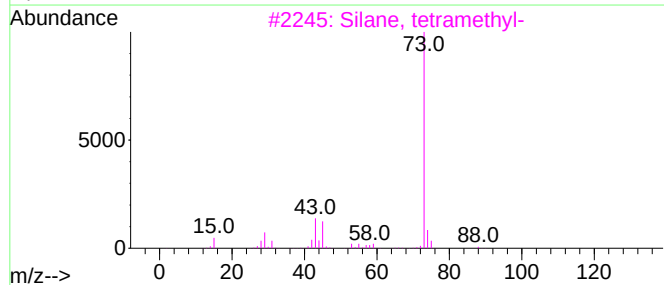
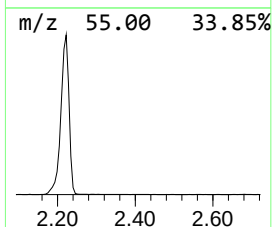
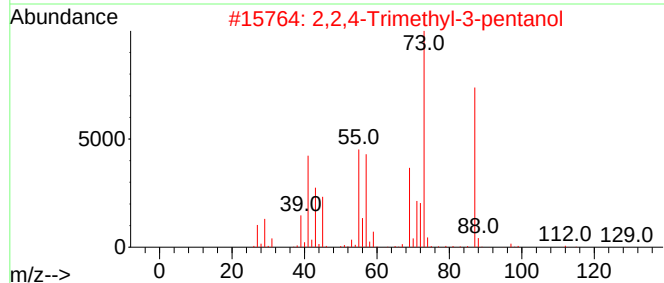
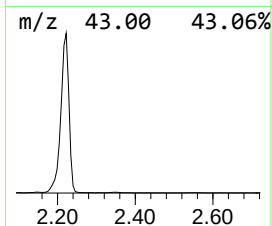
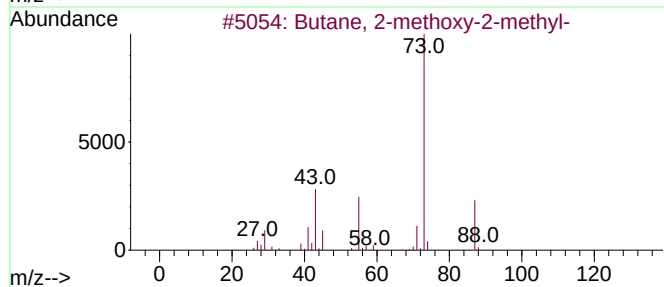
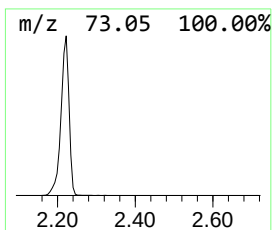
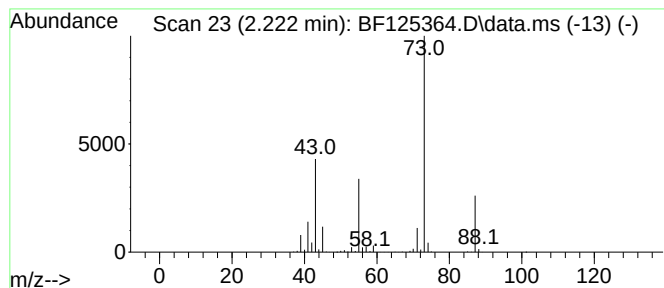
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	104.22 ng	4358440	1,4-Dichlorobenzene-d4	6.898

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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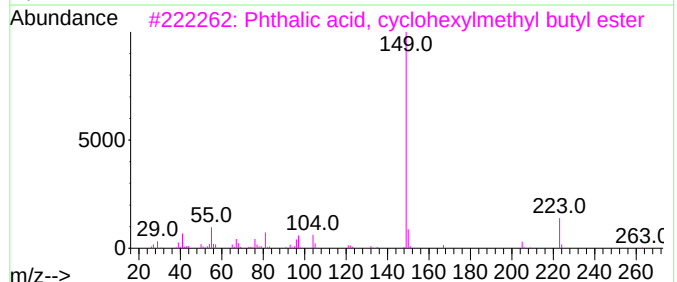
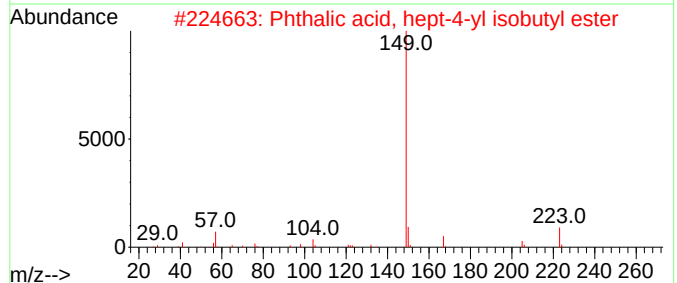
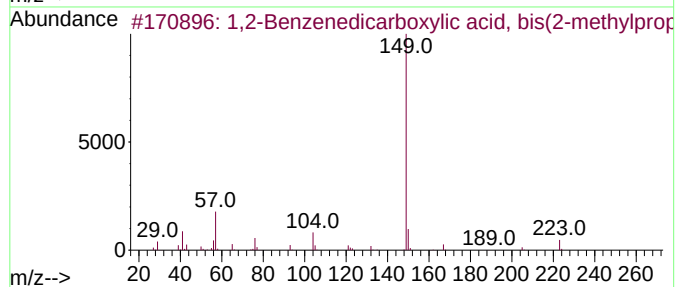
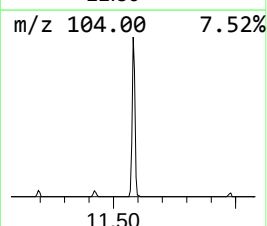
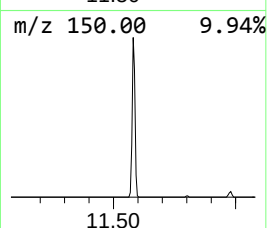
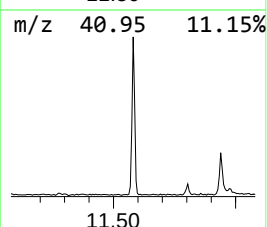
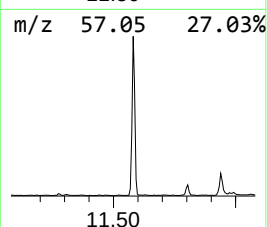
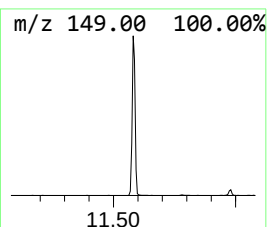
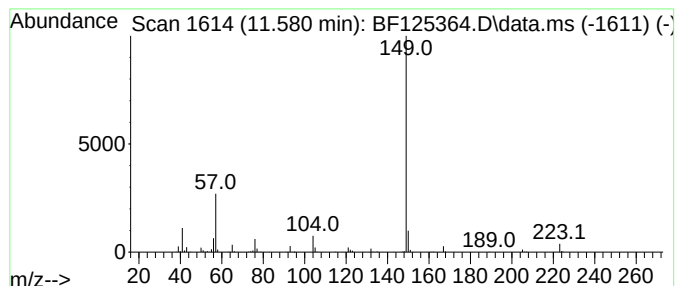
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Peak Number 2 1,2-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.580	21.05 ng	1124140	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	90
2			Phthalic acid, hept-4-yl isobuty...	320	C19H28O4	1000356-78-3	83
3			Phthalic acid, cyclohexylmethyl ...	318	C19H26O4	1000309-08-6	78
4			Phthalic acid, hex-3-yl isobutyl...	306	C18H26O4	1000356-95-4	78
5			1,2-Benzenedicarboxylic acid, bi...	250	C14H18O4	000605-45-8	78



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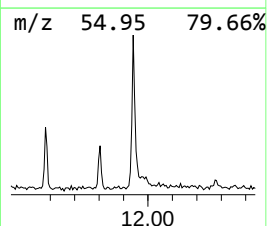
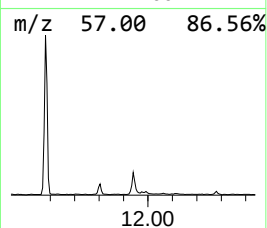
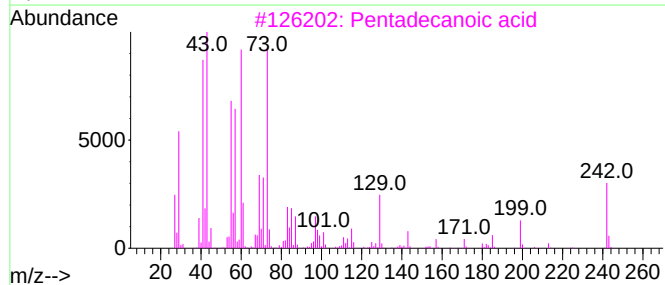
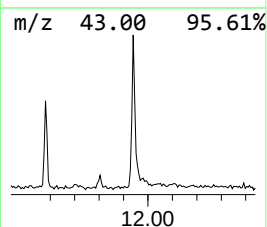
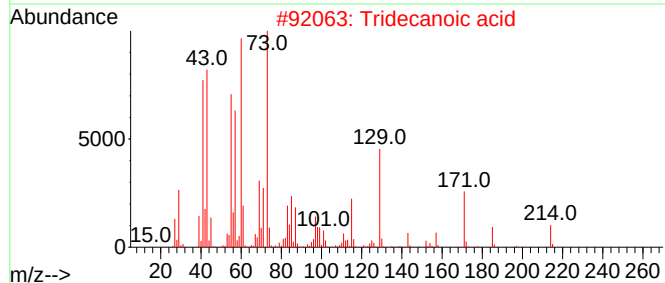
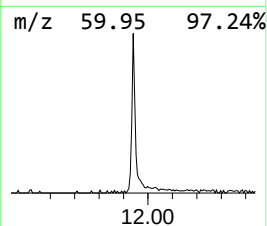
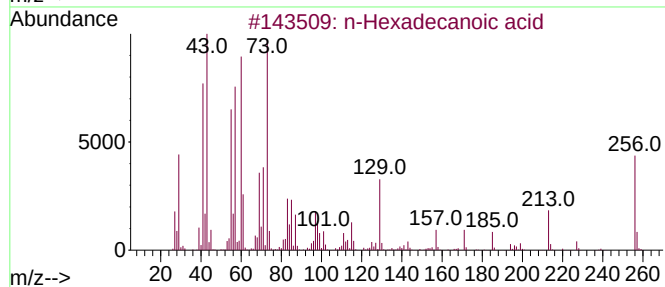
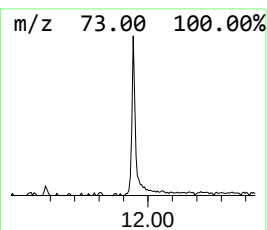
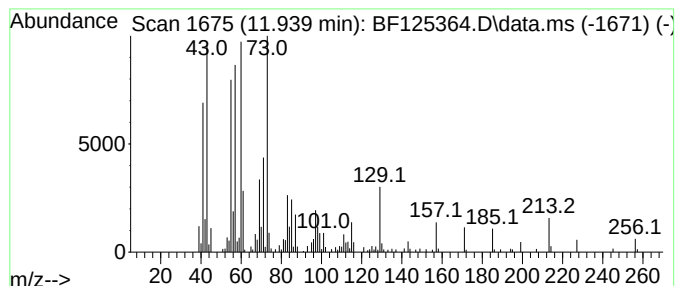
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	5.68 ng	303302	Phenanthrene-d10	11.422

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	80
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



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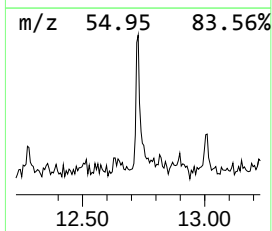
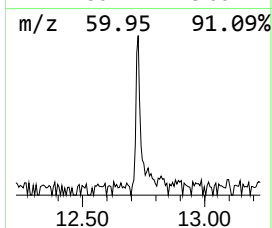
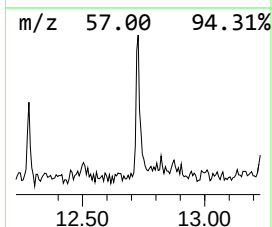
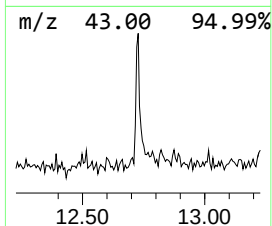
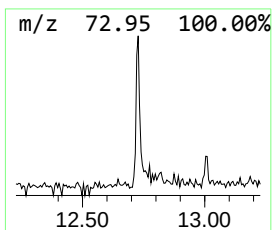
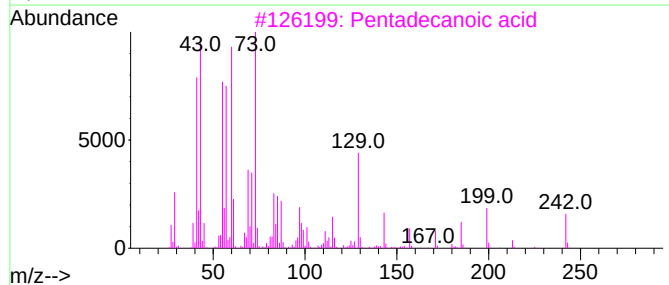
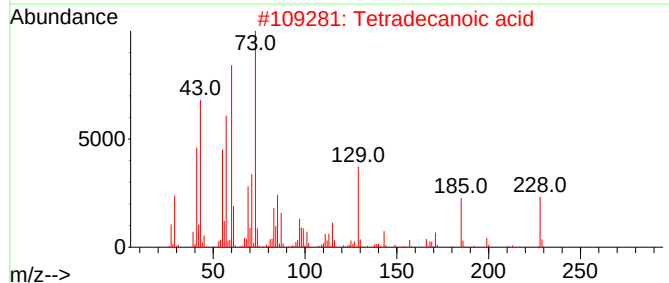
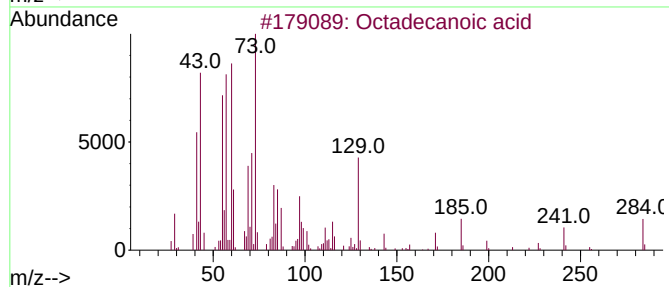
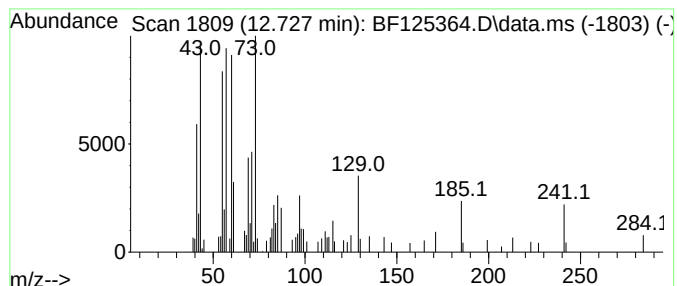
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.727	2.08 ng	110891	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	87
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58



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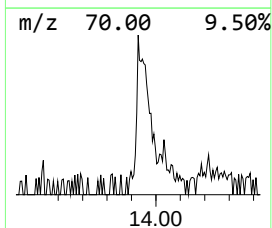
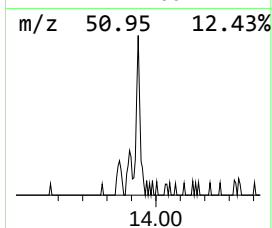
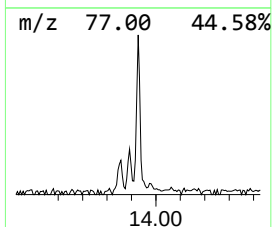
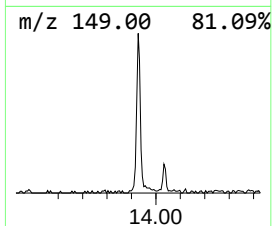
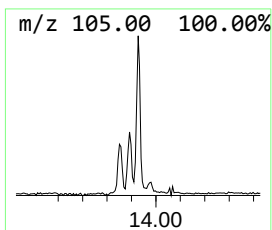
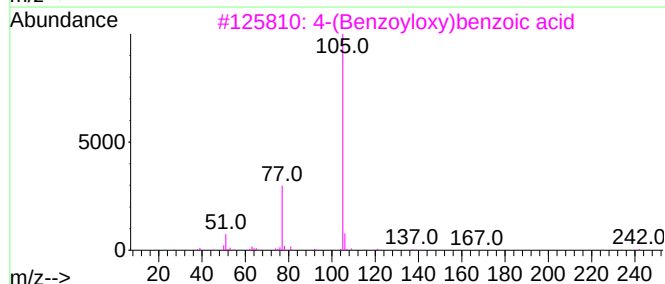
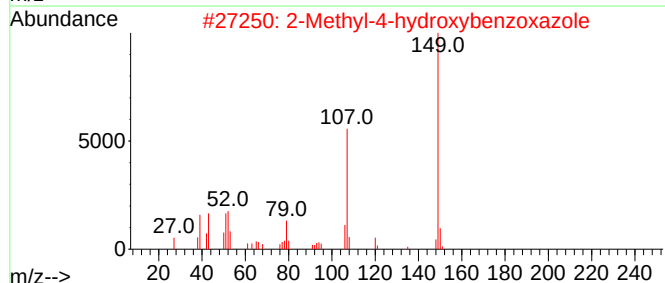
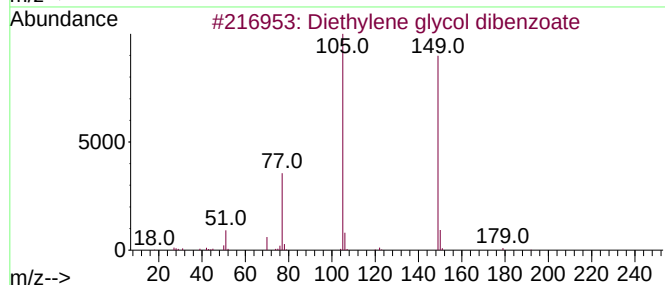
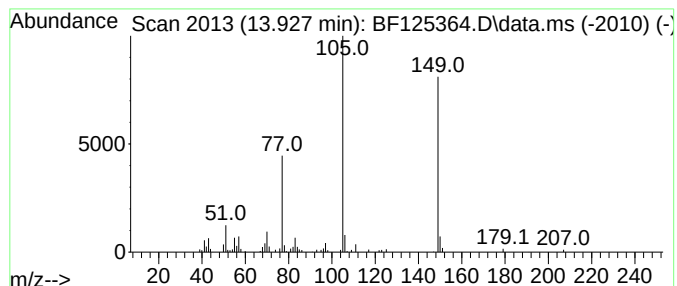
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	4.26 ng	163335	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
2			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43
3			4-(Benzoyloxy)benzoic acid	242	C14H10O4	028547-23-1	27
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	27
5			Phenylglyoxylic acid, isopropyl ...	192	C11H12O3	1000453-46-3	27



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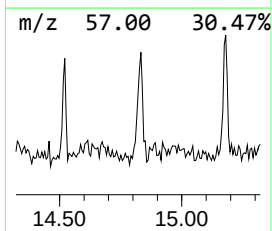
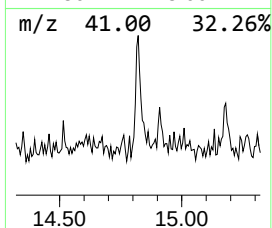
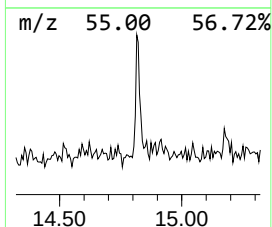
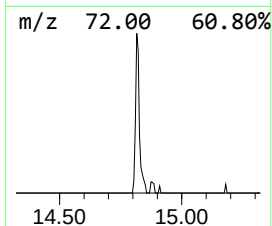
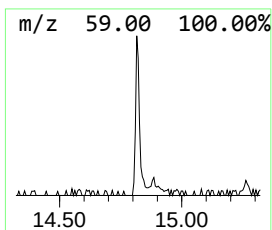
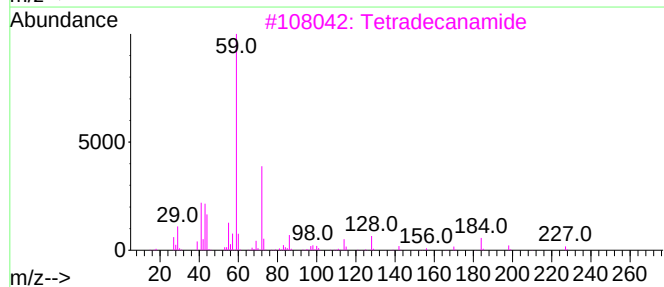
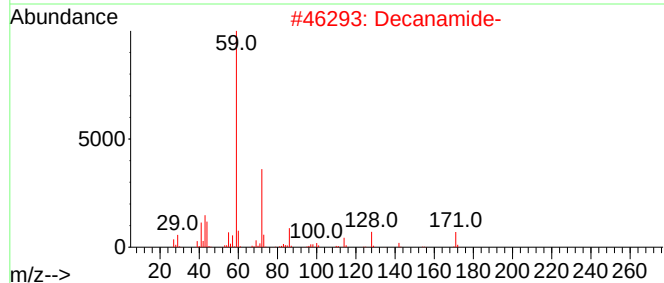
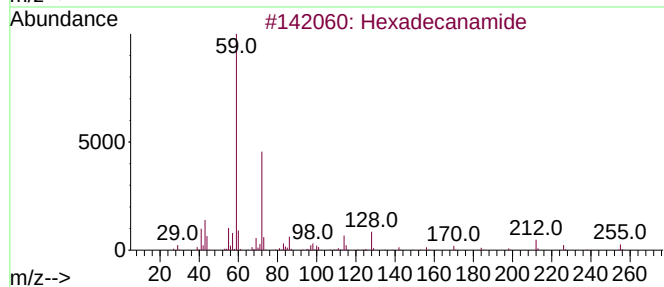
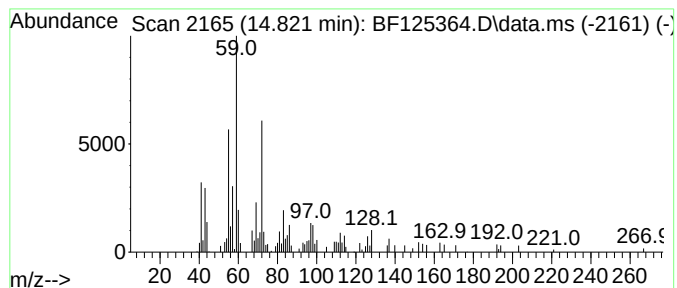
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	2.31 ng	100129	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanamide	255	C16H33NO	000629-54-9	59
2			Decanamide-	171	C10H21NO	002319-29-1	58
3			Tetradecanamide	227	C14H29NO	000638-58-4	53
4			Palmitoleamide	253	C16H31NO	106010-22-4	53
5			Dodecanamide	199	C12H25NO	001120-16-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090421\
Data File : BF125364.D
Acq On : 4 Sep 2021 12:23
Operator : JU/CG
Sample : M3648-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211058-SI-COMP-3-MODIFIED-EL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.222	104.2	ng	4358440	1	6.898	836396	20.0
1,2-Benzenedica...	11.580	21.1	ng	1124140	4	11.422	1067840	20.0
n-Hexadecanoic ...	11.939	5.7	ng	303302	4	11.422	1067840	20.0
Octadecanoic acid	12.727	2.1	ng	110891	4	11.422	1067840	20.0
Diethylene glyc...	13.927	4.3	ng	163335	5	14.063	766559	20.0
Hexadecanamide	14.821	2.3	ng	100129	6	15.557	867904	20.0