

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
 Data File : BF125230.D
 Acq On : 26 Aug 2021 17:52
 Operator : JU/CG
 Sample : M3547-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-4

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: BF125230.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	16	23	29	rVB	1594448	2064086	43.85%	5.664%
2	5.534	581	586	589	rBV	4709234	4409244	93.68%	12.099%
3	6.534	751	756	759	rBV	4223816	4319080	91.77%	11.851%
4	6.910	817	820	824	rBV	1414235	1215228	25.82%	3.334%
5	7.475	911	916	919	rBV	3101891	2832023	60.17%	7.771%
6	8.092	1018	1021	1033	rBV	174936	314875	6.69%	0.864%
7	8.192	1035	1038	1042	rVV	1663103	1553043	33.00%	4.261%
8	9.269	1216	1221	1224	rBV	5518829	4706617	100.00%	12.914%
9	9.951	1333	1337	1340	rBV	1964078	1739589	36.96%	4.773%
10	10.739	1466	1471	1474	rBV	3450307	3227726	68.58%	8.857%
11	11.433	1586	1589	1593	rBV	1901209	1765807	37.52%	4.845%
12	11.951	1673	1677	1682	rBV	494091	544636	11.57%	1.494%
13	12.651	1792	1796	1805	rBV	46012	58473	1.24%	0.160%
14	12.739	1807	1811	1820	rBV	189873	216434	4.60%	0.594%
15	13.021	1855	1859	1862	rBV	5124924	4414818	93.80%	12.114%
16	13.945	2012	2016	2030	rBV3	177254	459152	9.76%	1.260%
17	14.074	2035	2038	2042	rVB	1498116	1242677	26.40%	3.410%
18	14.833	2164	2167	2174	rBV2	98579	134902	2.87%	0.370%
19	15.568	2287	2292	2305	rVB2	906091	1226067	26.05%	3.364%

Sum of corrected areas: 36444477

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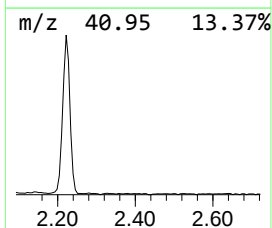
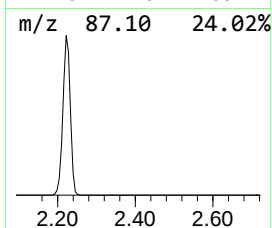
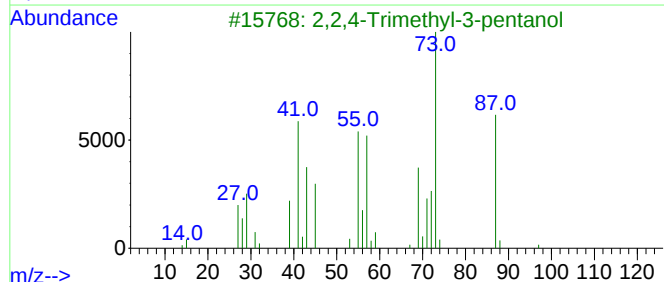
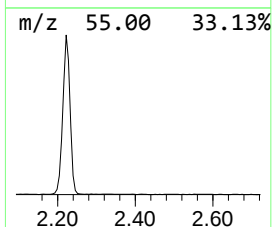
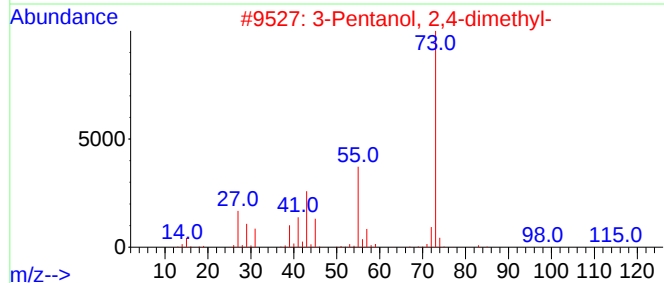
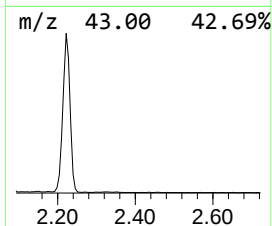
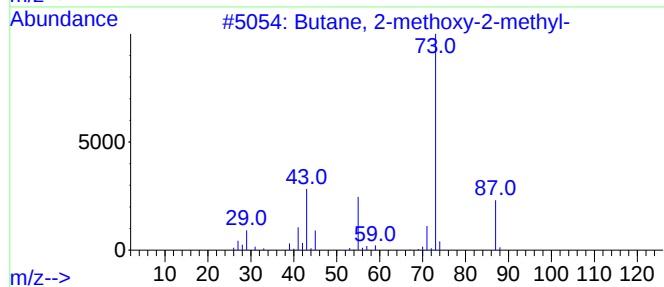
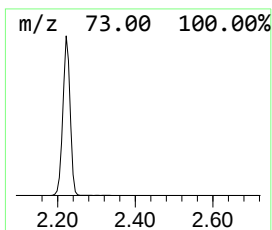
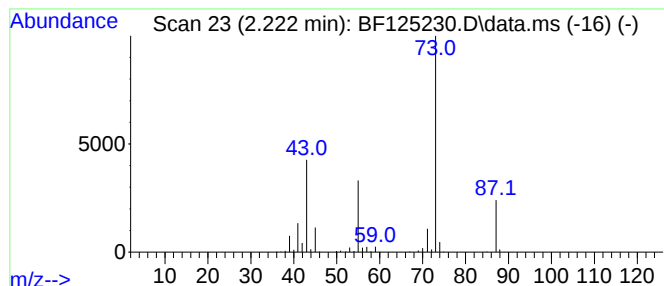
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	33.97 ng	2064090	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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37



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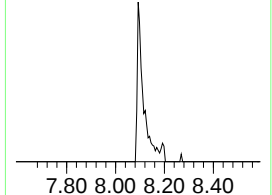
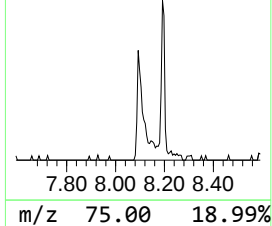
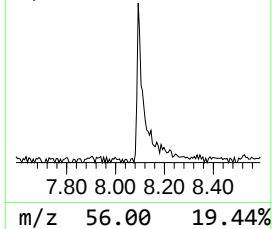
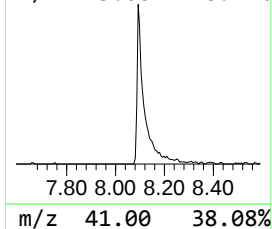
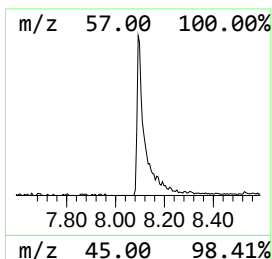
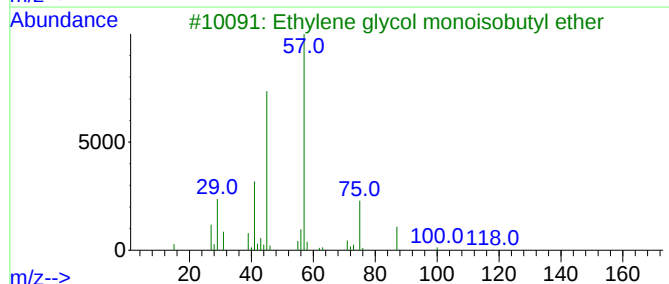
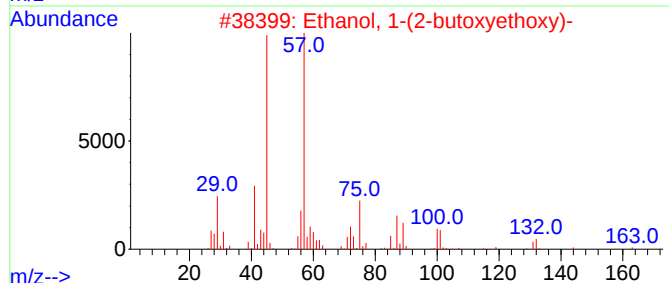
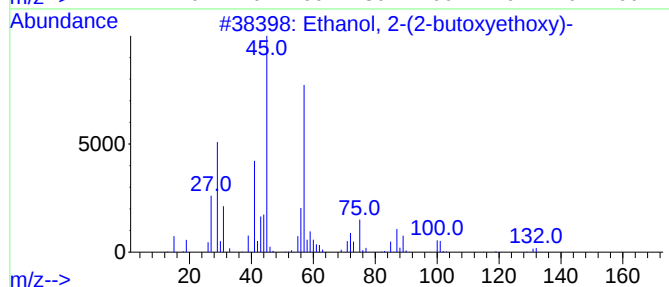
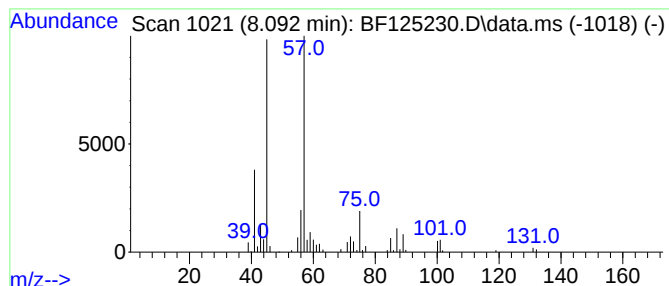
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	4.05 ng	314875	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	72
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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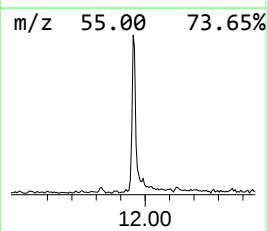
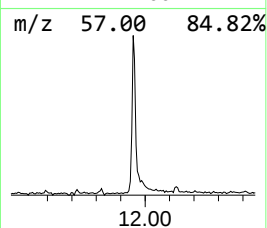
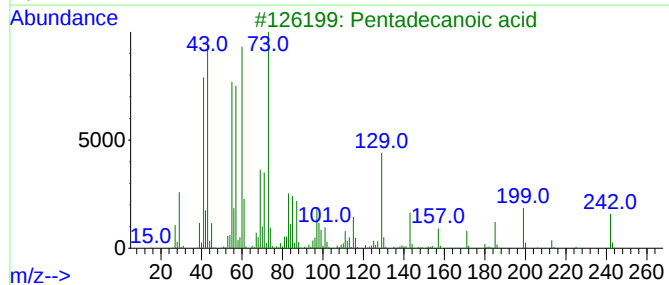
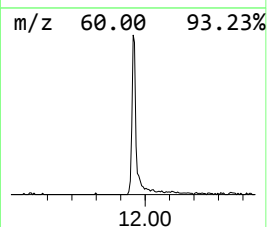
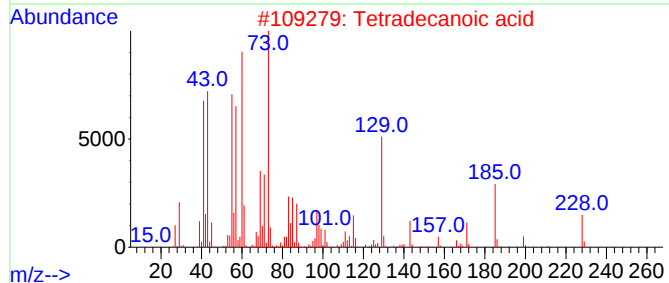
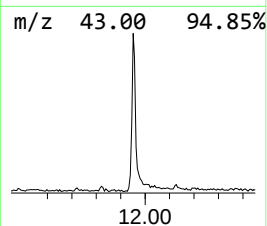
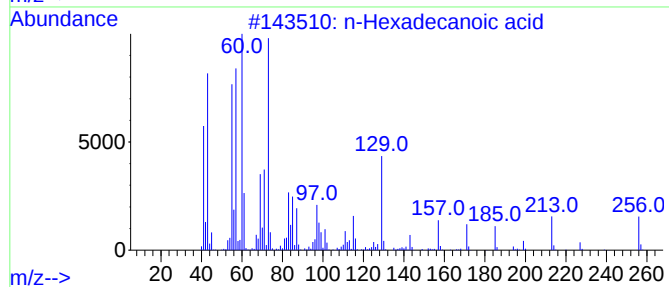
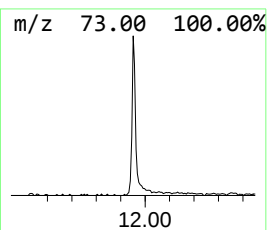
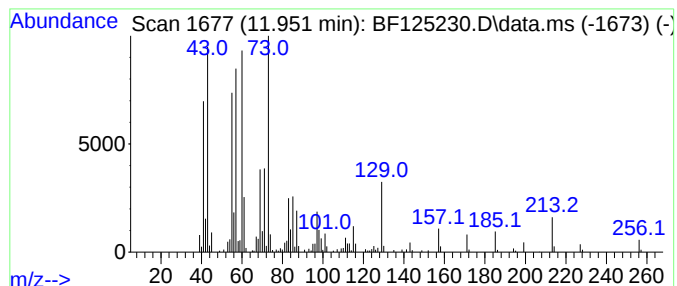
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	6.17 ng	544636	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	87
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	15



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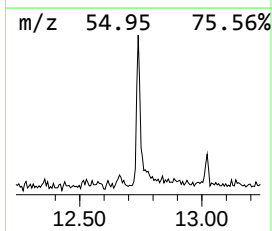
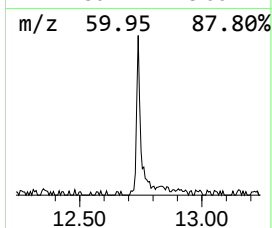
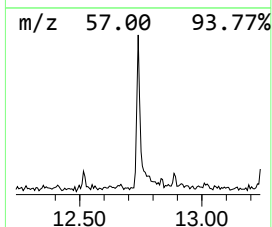
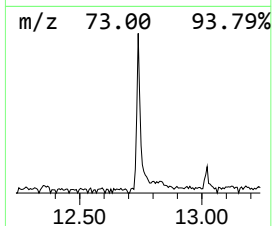
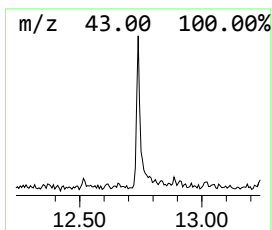
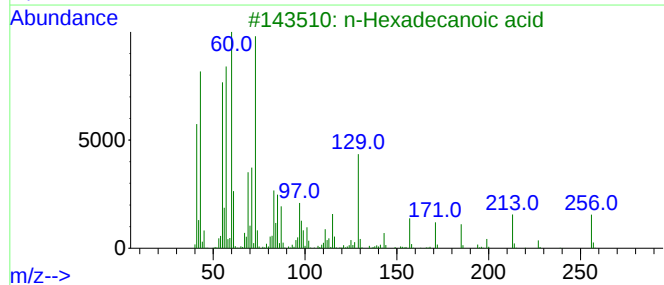
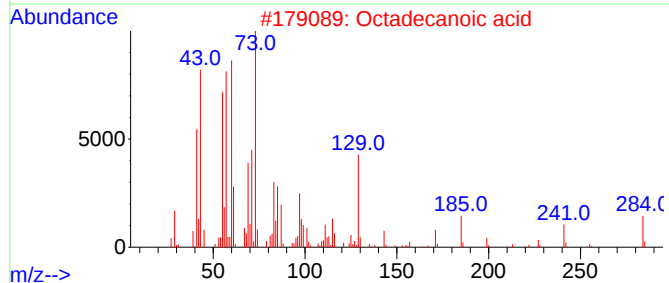
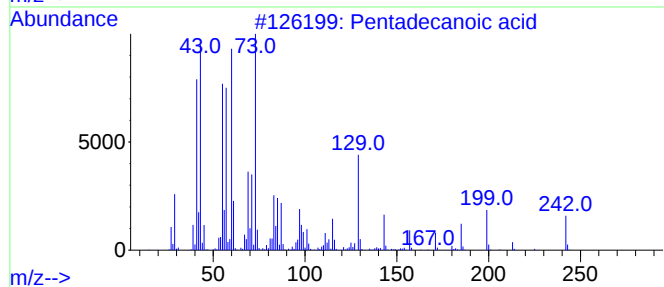
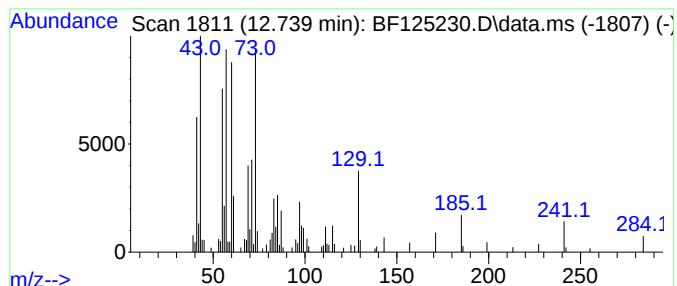
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Peak Number 4 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	2.45 ng	216434	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
2			Octadecanoic acid	284	C18H36O2	000057-11-4	94
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



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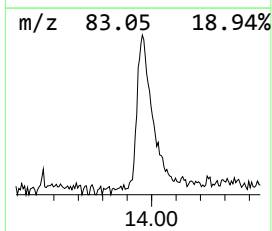
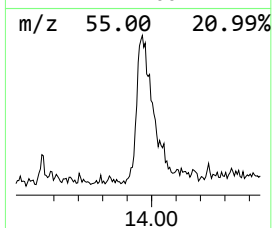
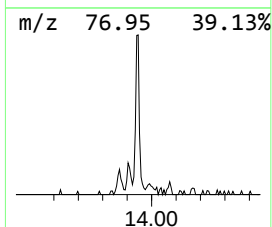
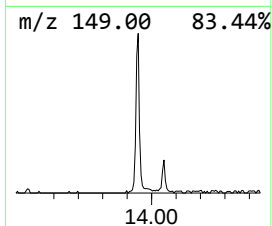
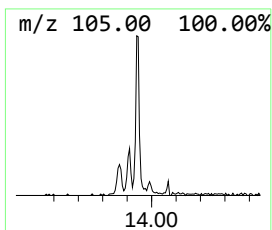
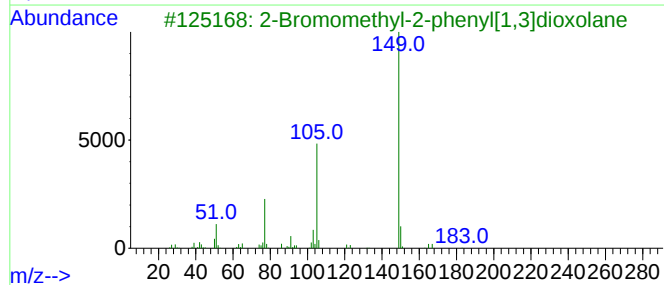
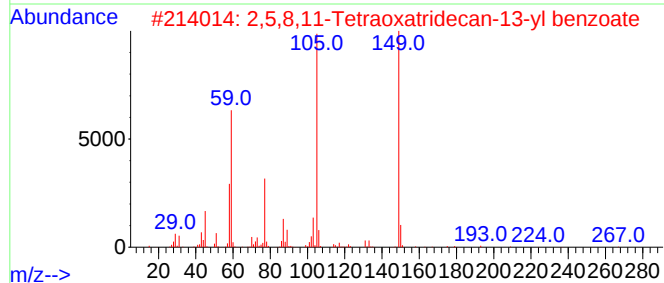
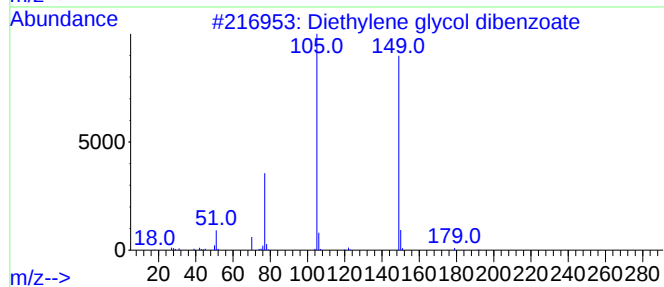
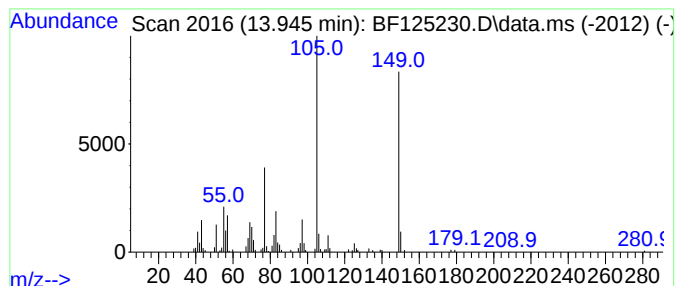
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	7.39 ng	459152	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
2			2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	64
3			2-Bromomethyl-2-phenyl[1,3]dioxo...	242	C10H11BrO2	003418-21-1	64
4			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	50
5			3-Benzoyl-2-t-butyl-4-(1-hydroxy...	333	C19H27NO4	1000194-87-3	27



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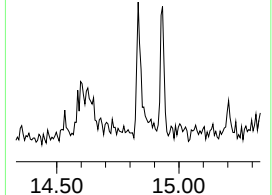
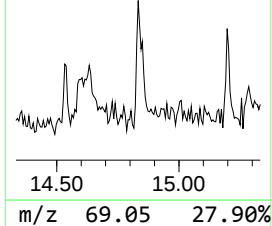
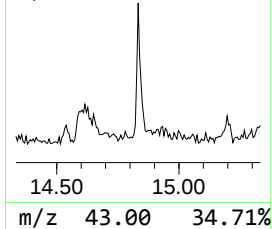
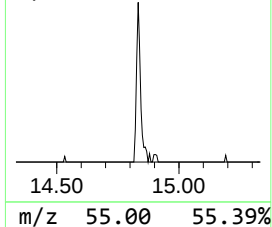
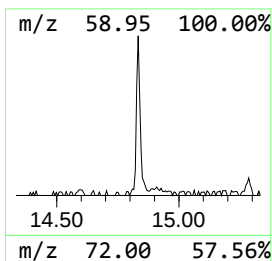
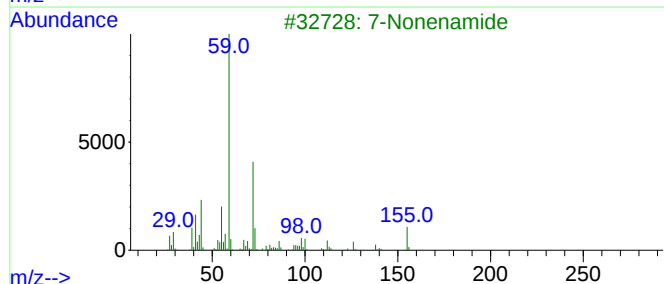
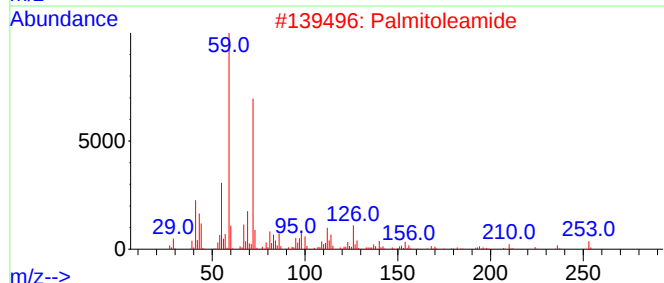
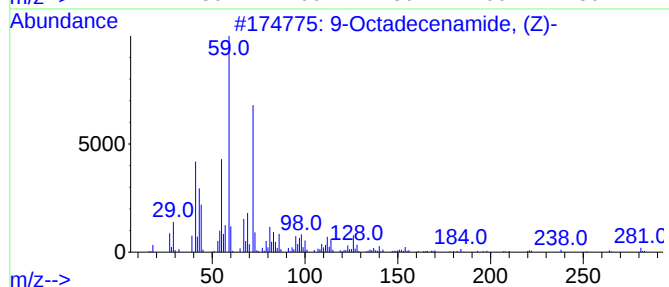
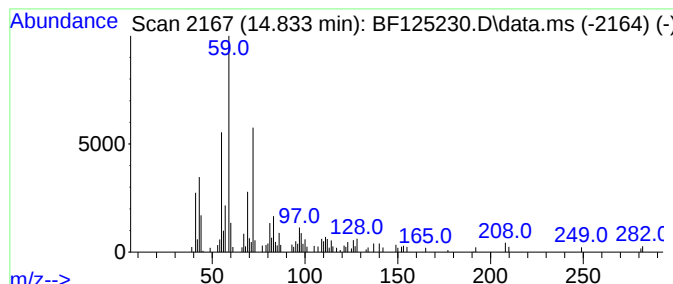
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TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	2.20 ng	134902	Perylene-d12	15.568

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2		Palmitoleamide	253	C16H31NO	106010-22-4	72
3		7-Nonenamide	155	C9H17NO	090949-53-4	68
4		Octanamide	143	C8H17NO	000629-01-6	53
5		Decanamide-	171	C10H21NO	002319-29-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
Data File : BF125230.D
Acq On : 26 Aug 2021 17:52
Operator : JU/CG
Sample : M3547-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-4

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	34.0	ng	2064090	1	6.910	1215230	20.0
Ethanol, 2-(2-b...	8.092	4.0	ng	314875	2	8.198	1553040	20.0
n-Hexadecanoic ...	11.951	6.2	ng	544636	4	11.433	1765810	20.0
Pentadecanoic acid	12.739	2.5	ng	216434	4	11.433	1765810	20.0
Diethylene glyc...	13.945	7.4	ng	459152	5	14.074	1242680	20.0
9-Octadecenamid...	14.833	2.2	ng	134902	6	15.568	1226070	20.0