

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062421\
 Data File : BF124446.D
 Acq On : 24 Jun 2021 16:57
 Operator : JU/CG
 Sample : M2835-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-075

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-BF062321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124446.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.922	480	482	490	rBV2	11919	15341	1.42%	0.220%
2	5.340	549	553	567	rBV	925402	875479	80.92%	12.578%
3	6.369	724	728	737	rBV	993836	893528	82.59%	12.837%
4	6.716	784	787	792	rBV	287891	218482	20.20%	3.139%
5	7.286	880	884	887	rBV	638638	544346	50.32%	7.821%
6	7.910	987	990	999	rBV	228958	211090	19.51%	3.033%
7	7.998	1002	1005	1009	rVB	354798	281474	26.02%	4.044%
8	9.080	1185	1189	1192	rBV	1439353	1081858	100.00%	15.543%
9	9.757	1300	1304	1307	rBV	442136	342767	31.68%	4.925%
10	10.551	1435	1439	1444	rBV	650406	582813	53.87%	8.373%
11	11.245	1553	1557	1560	rBV	397781	322284	29.79%	4.630%
12	11.639	1620	1624	1631	rVB3	26845	25220	2.33%	0.362%
13	11.780	1645	1648	1654	rBV5	37041	47228	4.37%	0.679%
14	12.498	1767	1770	1772	rBV4	17379	14077	1.30%	0.202%
15	12.692	1799	1803	1805	rBV4	9634	15647	1.45%	0.225%
16	12.833	1823	1827	1830	rBV	930994	737172	68.14%	10.591%
17	13.739	1979	1981	1982	rBV2	20066	16190	1.50%	0.233%
18	13.763	1982	1985	1987	rBV4	35886	43120	3.99%	0.620%
19	13.892	2004	2007	2011	rBV	277050	244750	22.62%	3.516%
20	14.221	2061	2063	2064	rBV2	24324	18434	1.70%	0.265%
21	14.239	2064	2066	2067	rBV2	22560	13703	1.27%	0.197%
22	14.980	2190	2192	2197	rVB5	52546	64185	5.93%	0.922%
23	15.333	2248	2252	2258	rVB	176378	223413	20.65%	3.210%
24	15.833	2335	2337	2341	rVB5	21462	18341	1.70%	0.264%
25	17.098	2548	2552	2556	rBV7	18104	32557	3.01%	0.468%
26	17.192	2566	2568	2571	rBV4	18048	14529	1.34%	0.209%
27	18.227	2742	2744	2751	rVB8	34006	62345	5.76%	0.896%

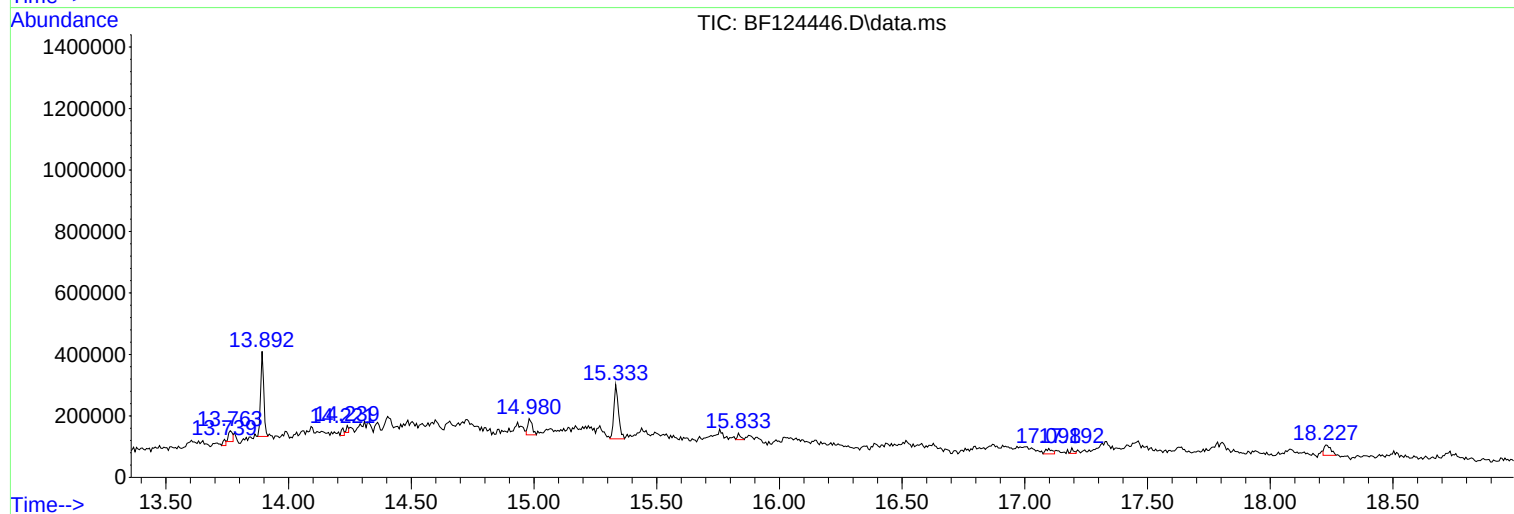
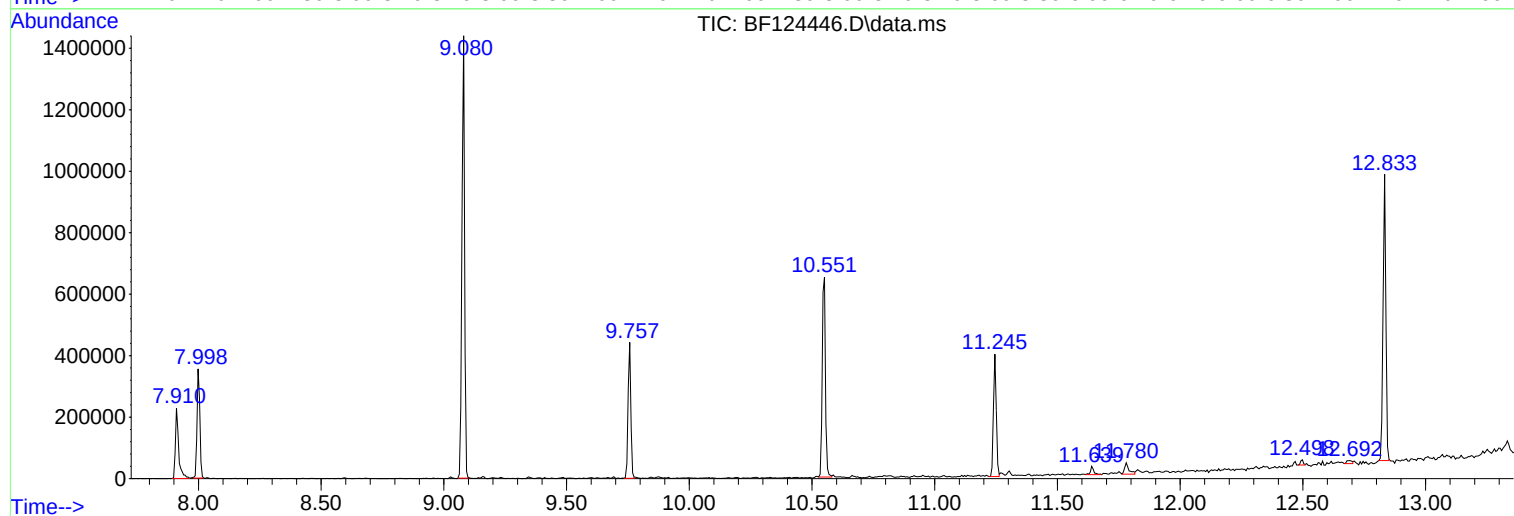
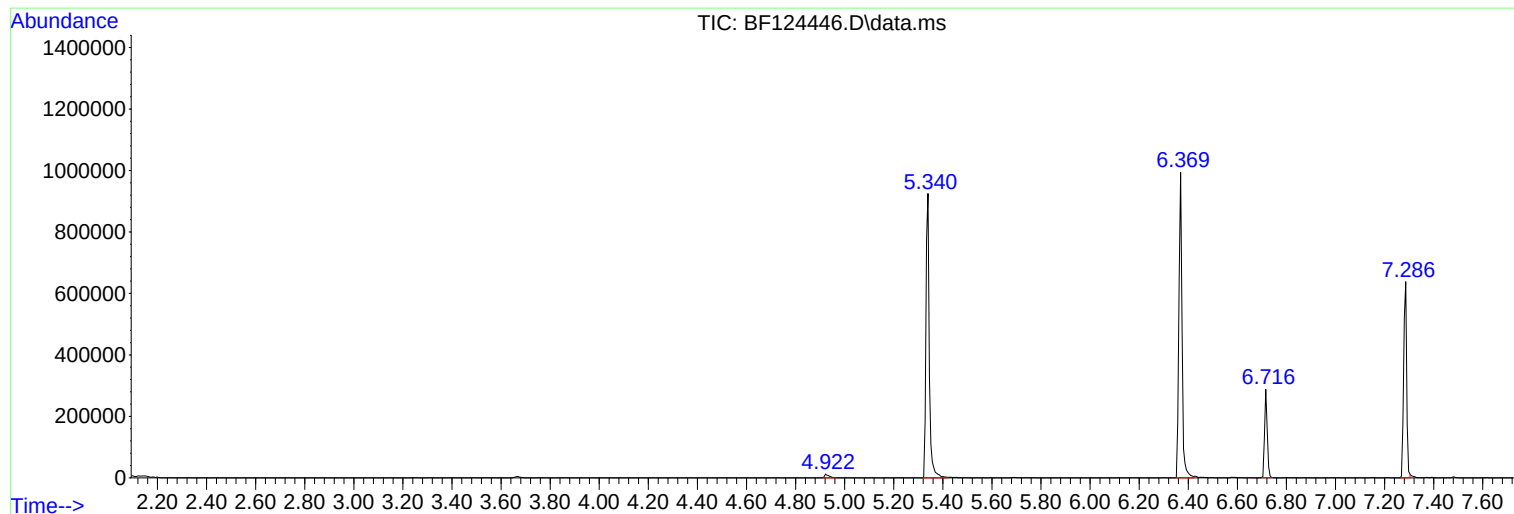
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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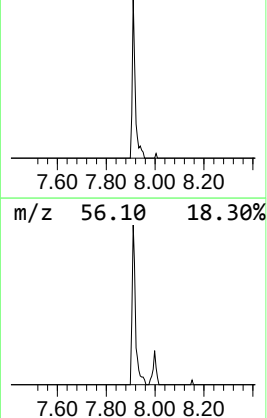
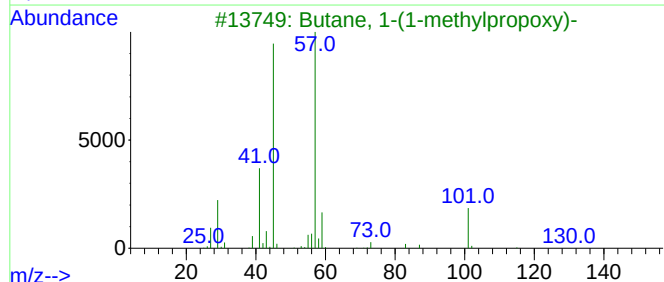
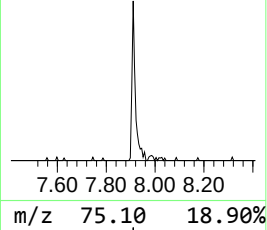
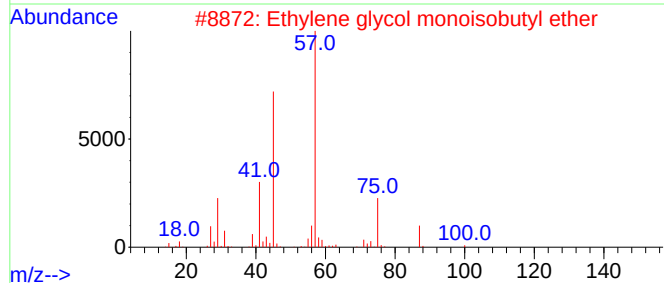
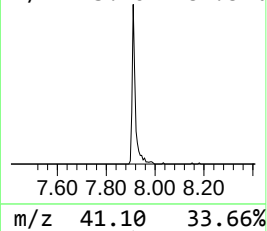
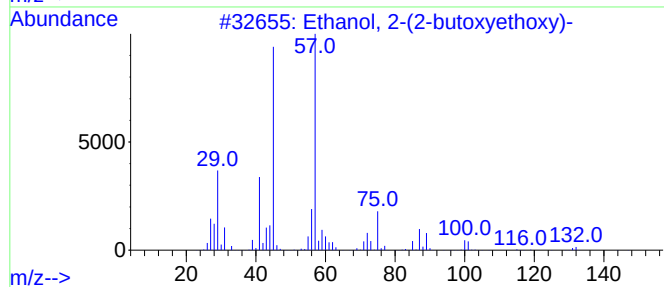
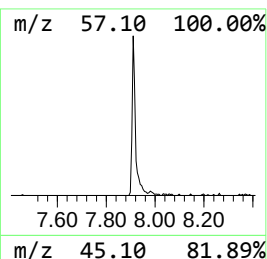
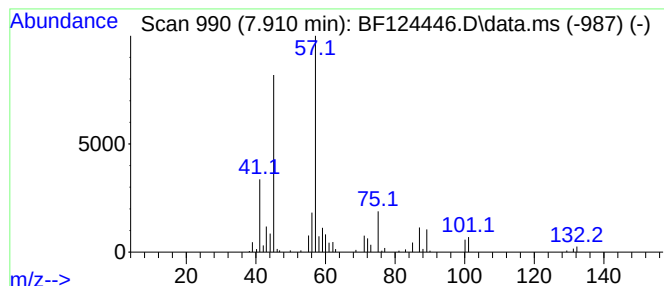
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Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.910	15.00 ng	211090	Naphthalene-d8	7.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5			2-Propanol, 1-(2-butoxyethoxy)-	176	C9H20O3	000124-16-3	50



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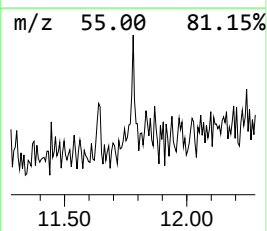
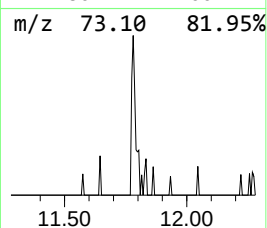
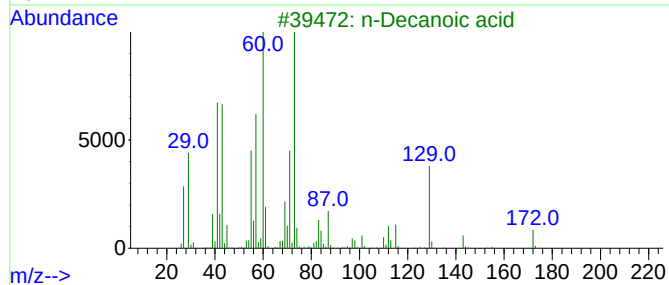
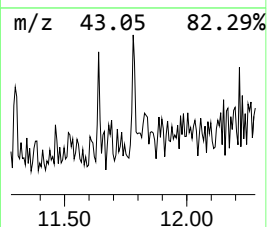
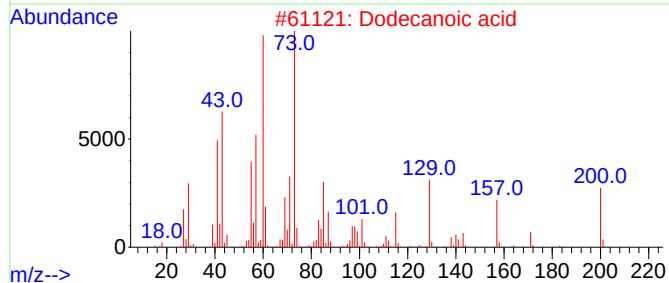
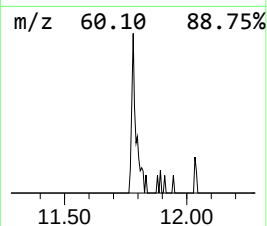
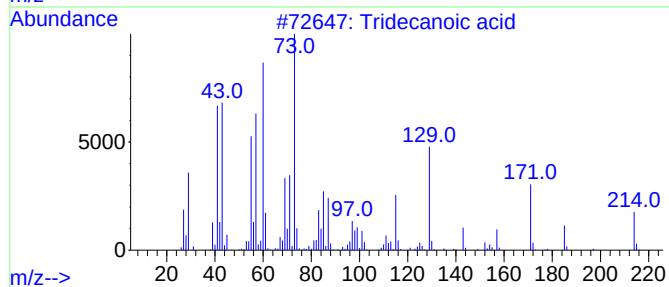
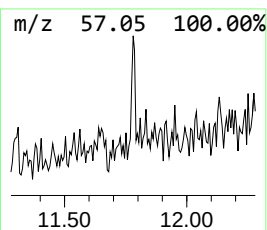
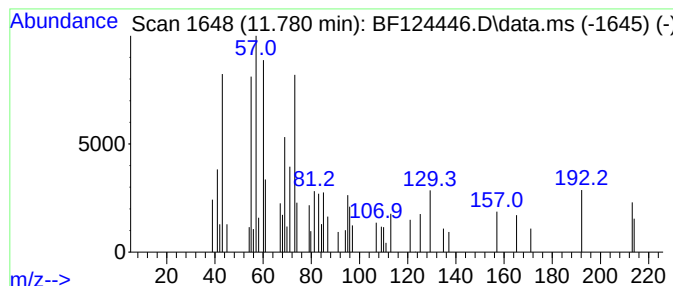
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Peak Number 2 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	2.93 ng	47228	Phenanthrene-d10	11.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	70
2			Dodecanoic acid	200	C12H24O2	000143-07-7	52
3			n-Decanoic acid	172	C10H20O2	000334-48-5	47
4			Undecanoic acid	186	C11H22O2	000112-37-8	47
5			Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	10



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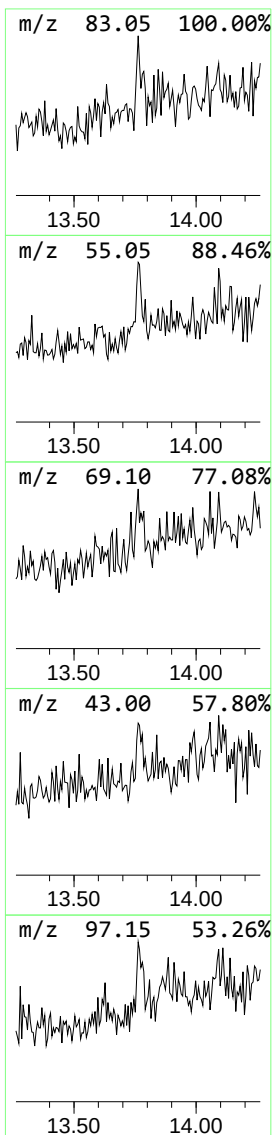
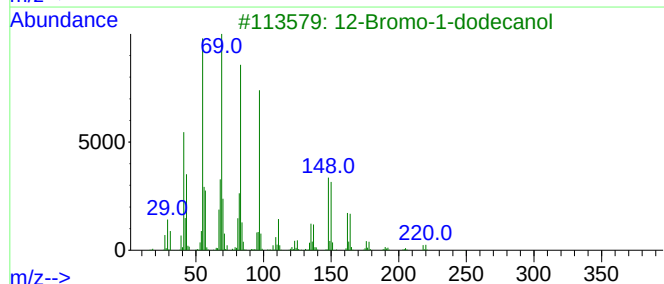
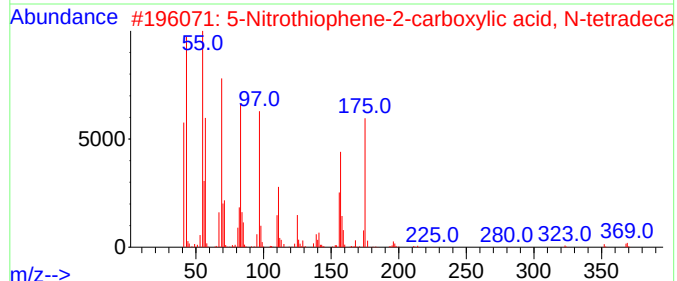
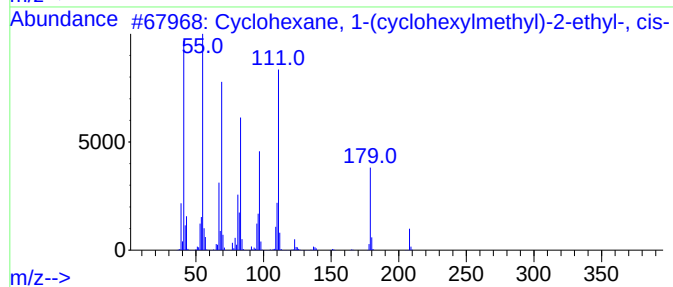
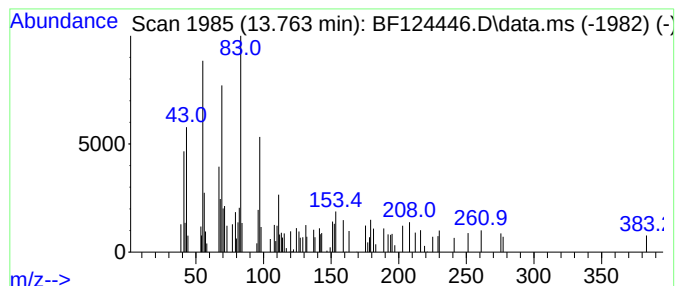
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Peak Number 3 Cyclohexane, 1-(cyclohexylm... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.762	3.52 ng	43120	Chrysene-d12	13.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-(cyclohexylmethyl...)	208	C15H28	054934-93-9	58
2			5-Nitrothiophene-2-carboxylic ac...	369	C19H31NO4S	1000253-28-2	47
3			12-Bromo-1-dodecanol	264	C12H25BrO	003344-77-2	46
4			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	46
5			Phosphetane, 1-chloro-2,2,3,4,4-...	194	C8H16ClOP	029276-11-7	38



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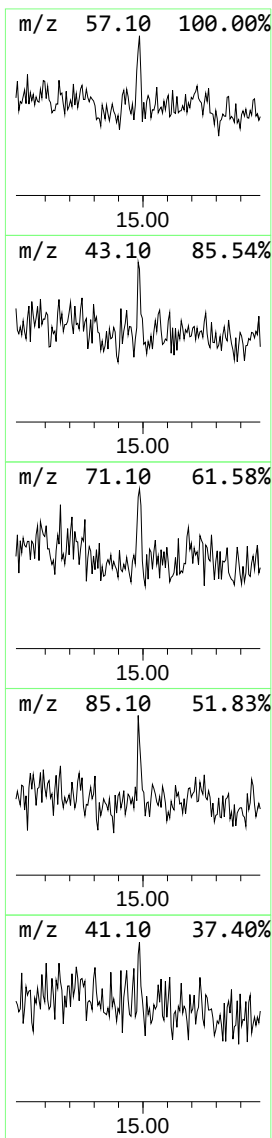
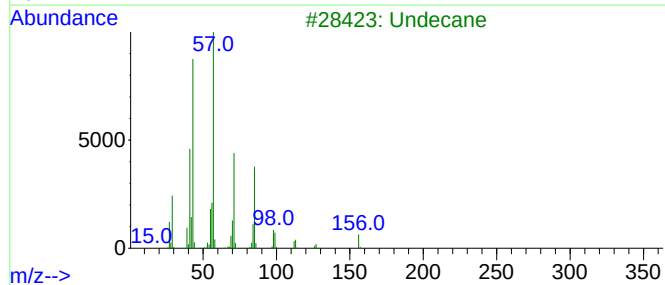
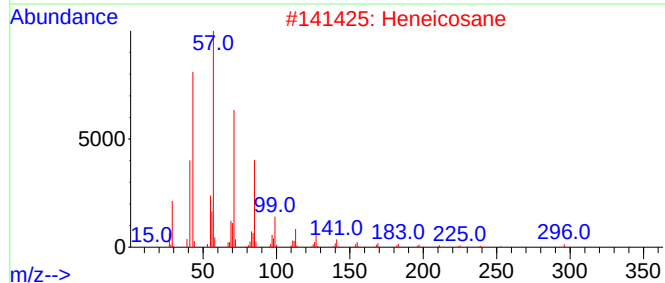
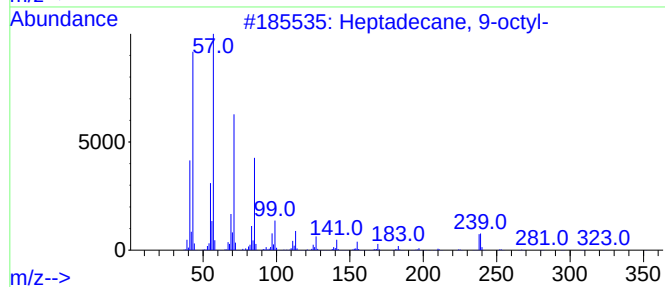
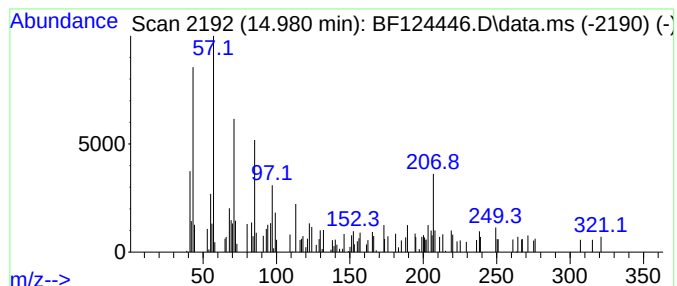
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Peak Number 4 unknown14.980 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.980	5.75 ng	64185	Perylene-d12	15.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	43
2			Heneicosane	296	C21H44	000629-94-7	38
3			Undecane	156	C11H24	001120-21-4	38
4			Eicosane	282	C20H42	000112-95-8	38
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	38



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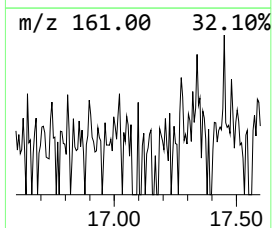
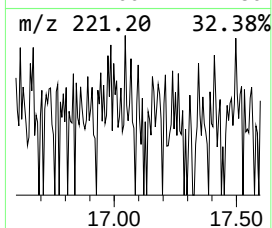
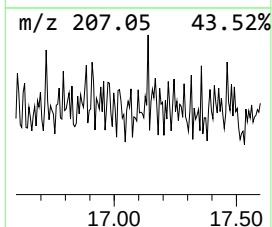
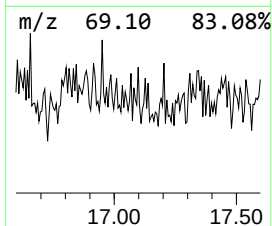
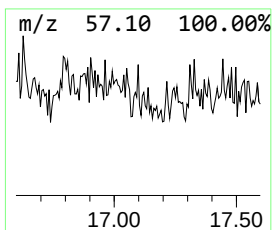
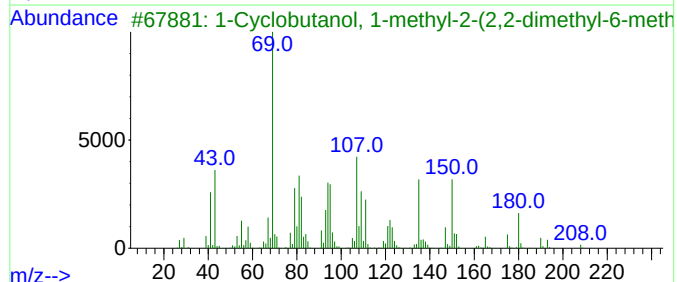
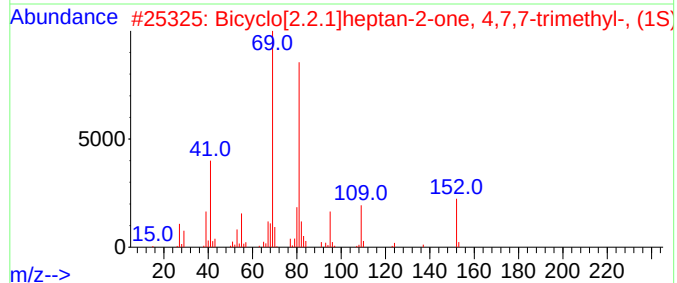
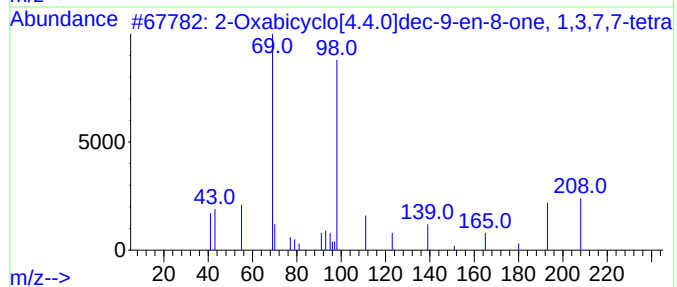
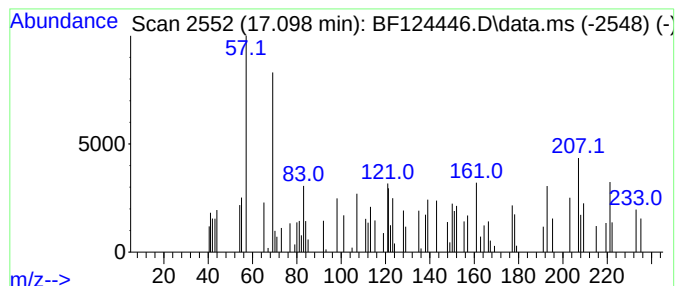
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Peak Number 5 unknown17.098 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.098	2.91 ng	32557	Perylene-d12	15.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Oxabicyclo[4.4.0]dec-9-en-8-on...	208	C13H20O2	122723-58-4	16
2			Bicyclo[2.2.1]heptan-2-one, 4,7,...	152	C10H16O	010292-98-5	14
3			1-Cyclobutanol, 1-methyl-2-(2,2-...	208	C14H24O	1000197-21-8	14
4			8-Hexadecanol	242	C16H34O	019781-83-0	14
5			6-Methyl-8-oxo-6,7,8,9-tetrahydr...	221	C11H18N4O4	134076-69-0	12



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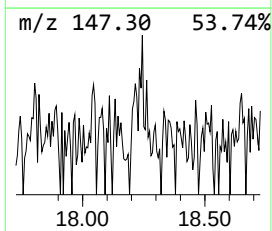
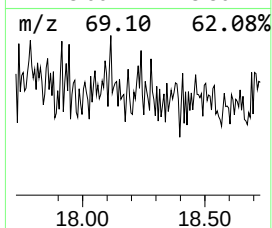
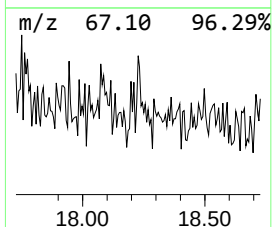
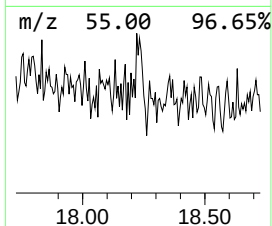
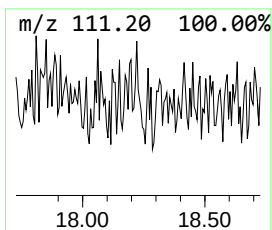
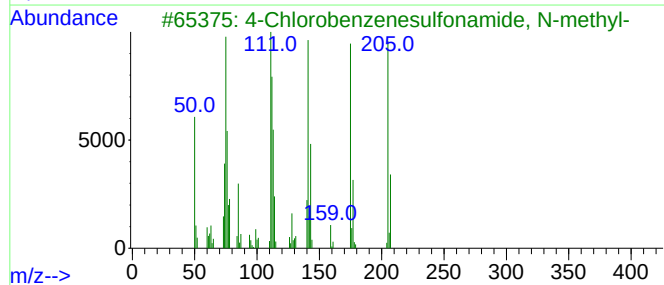
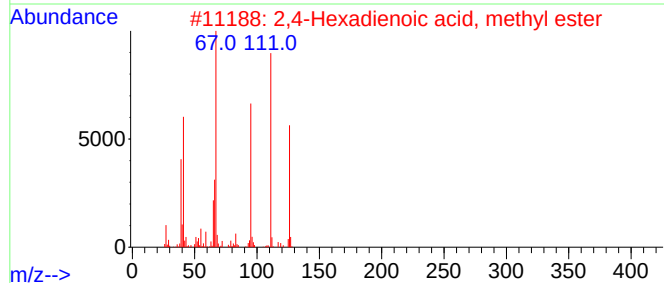
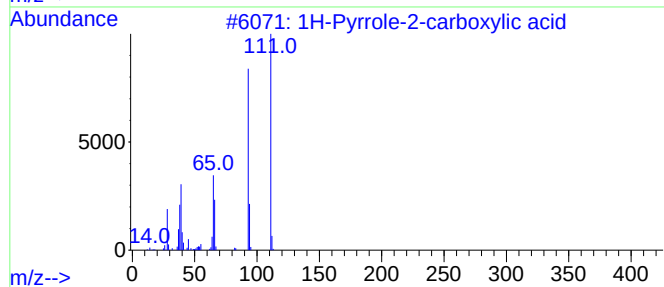
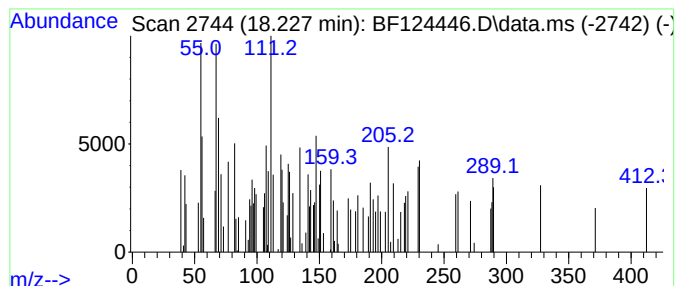
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Peak Number 6 unknown18.227 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.227	5.58 ng	62345	Perylene-d12	15.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Pyrrole-2-carboxylic acid	111	C5H5NO2	000634-97-9	25
2			2,4-Hexadienoic acid, methyl ester	126	C7H10O2	001515-80-6	25
3			4-Chlorobenzenesulfonamide, N-me...	205	C7H8ClNO2S	006333-79-5	15
4			Benzo[1,2,5]oxadiazol-5-ylthioph...	230	C11H6N2O2S	226090-73-9	14
5			1,2,4-Triazolidin-3-thione, 5-me...	289	C14H15N3S2	346459-14-1	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062421\
Data File : BF124446.D
Acq On : 24 Jun 2021 16:57
Operator : JU/CG
Sample : M2835-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-075

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	7.910	15.0	ng	211090	2	7.998	281474	20.0
Tridecanoic acid	11.780	2.9	ng	47228	4	11.245	322284	20.0
Cyclohexane, 1-...	13.762	3.5	ng	43120	5	13.892	244750	20.0
unknown14.980	14.980	5.8	ng	64185	6	15.333	223413	20.0
unknown17.098	17.098	2.9	ng	32557	6	15.333	223413	20.0
unknown18.227	18.227	5.6	ng	62345	6	15.333	223413	20.0