

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
 Data File : BF124173.D
 Acq On : 8 Jun 2021 10:17
 Operator : JU/CG
 Sample : PB136847BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB136847BL

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-BF060321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124173.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	8	16	21	rBB	57228	75220	3.01%	0.591%
2	5.498	575	580	583	rBV	1557432	1526351	61.04%	12.000%
3	6.504	746	751	754	rBV	1381011	1502435	60.08%	11.812%
4	6.857	808	811	815	rBV	352364	284045	11.36%	2.233%
5	7.428	902	908	910	rBV	932670	1036696	41.46%	8.151%
6	8.140	1025	1029	1033	rBV	396696	367466	14.70%	2.889%
7	9.222	1207	1213	1216	rBV	2415896	2099167	83.95%	16.504%
8	9.898	1324	1328	1332	rBV	590861	466955	18.67%	3.671%
9	10.692	1458	1463	1466	rBV	1674875	1486068	59.43%	11.684%
10	11.386	1577	1581	1584	rBV	594263	485307	19.41%	3.816%
11	12.980	1846	1852	1855	rBV	2798767	2500530	100.00%	19.660%
12	13.827	1983	1996	2000	rBV7	17648	61714	2.47%	0.485%
13	14.033	2026	2031	2034	rBV	411924	390686	15.62%	3.072%
14	15.510	2275	2282	2290	rBV	216208	308491	12.34%	2.425%
15	17.074	2532	2548	2549	rBV9	42075	100728	4.03%	0.792%
16	17.804	2664	2672	2676	rBV6	12594	27318	1.09%	0.215%

Sum of corrected areas: 12719177

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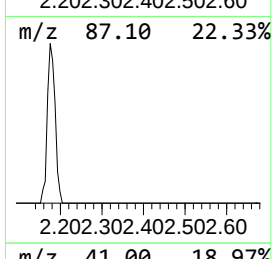
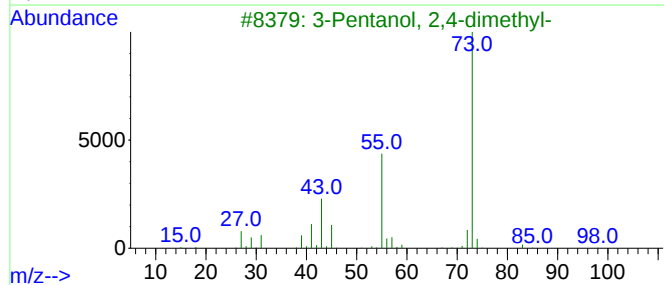
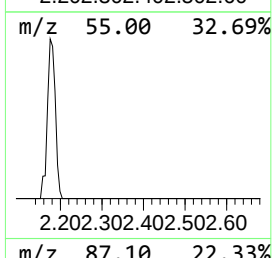
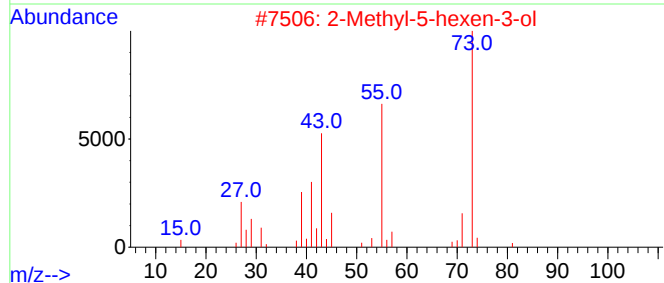
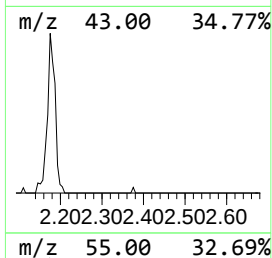
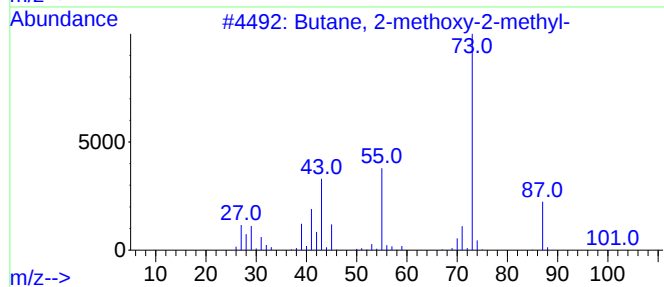
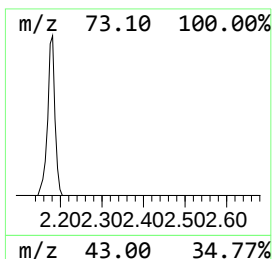
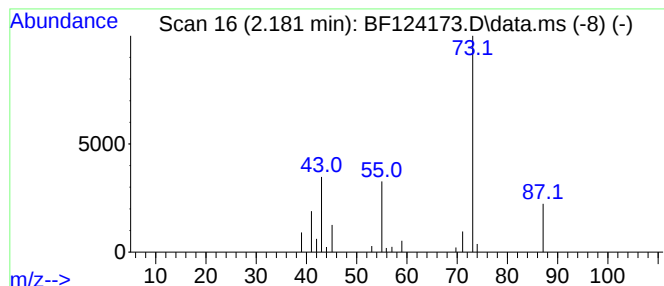
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
2.181	5.30 ng	75220	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
4			1,4-Butanediamine	88	C4H12N2	000110-60-1	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5



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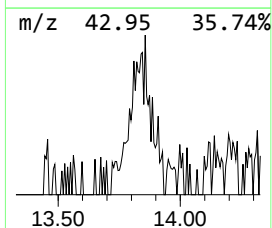
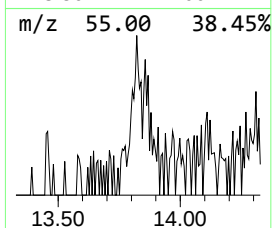
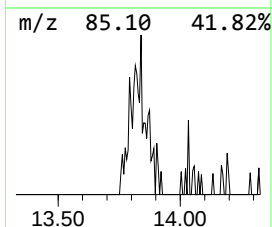
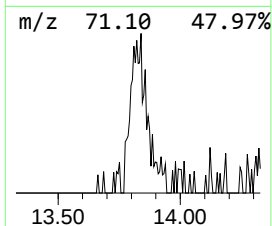
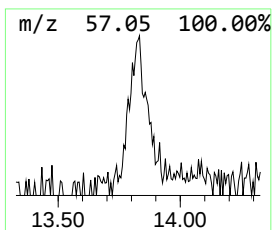
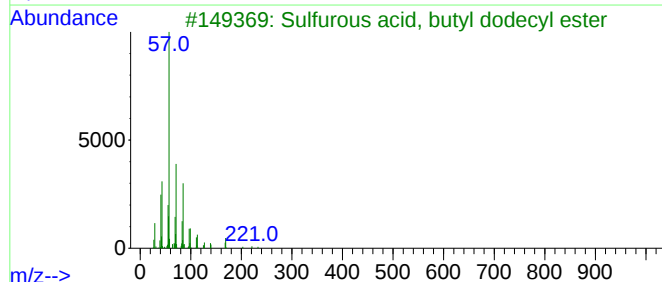
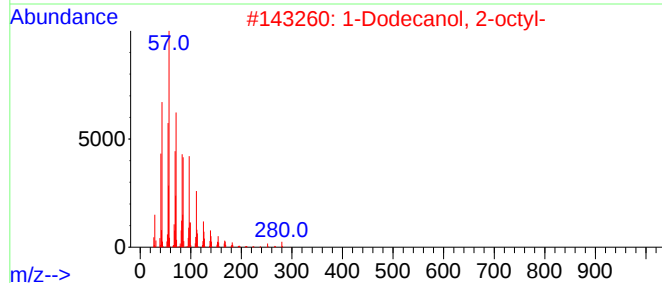
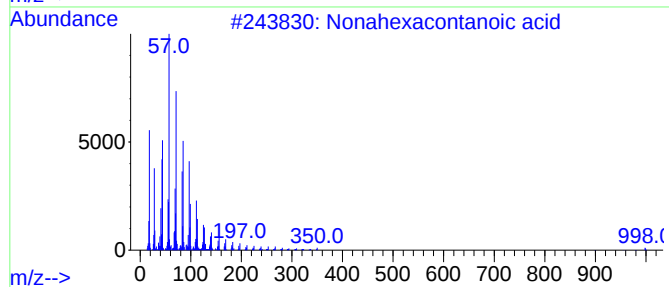
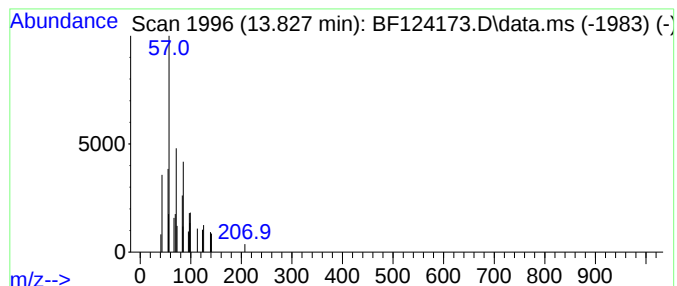
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Peak Number 2 Nonaheptacontanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	3.16 ng	61714	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonaheptacontanoic acid	999	C69H138O2	040710-32-5	72
2			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	53
3			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	53
4			Heptacosane	380	C27H56	000593-49-7	50
5			Heptadecane	240	C17H36	000629-78-7	50



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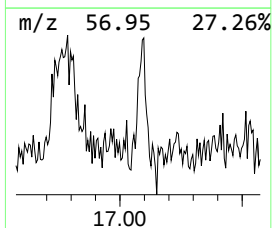
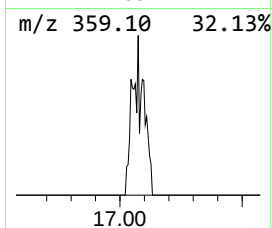
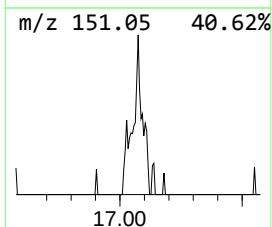
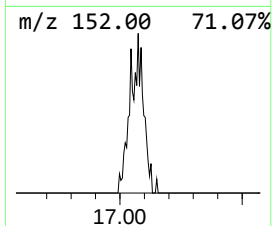
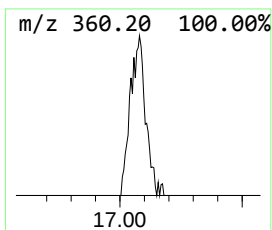
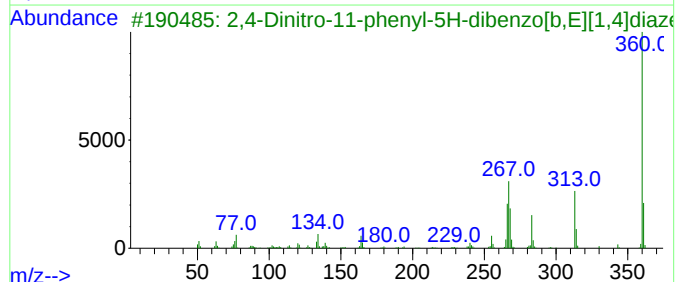
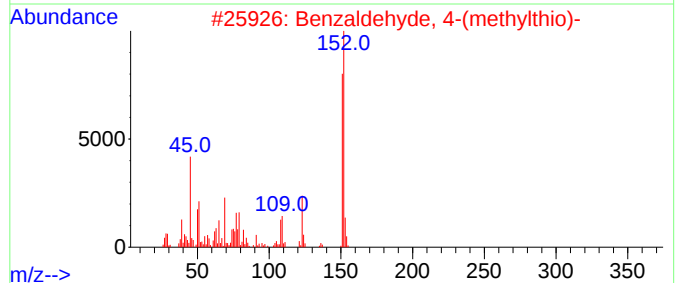
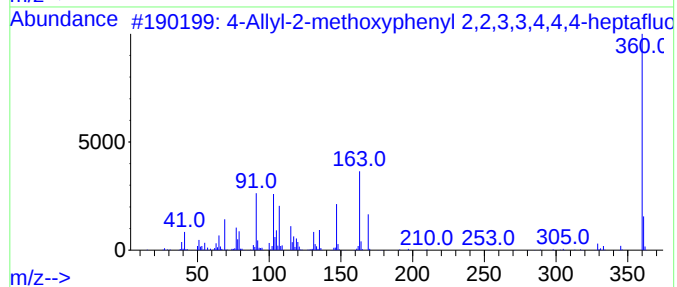
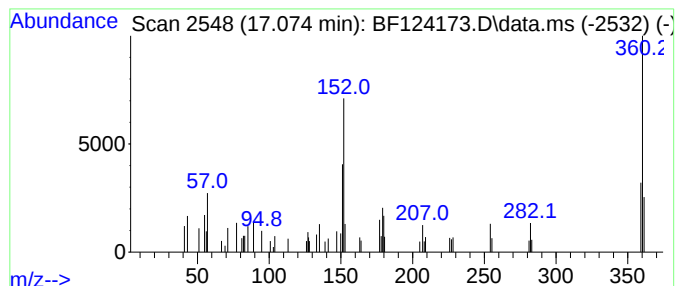
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown17.07 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.074	6.53 ng	100728	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Allyl-2-methoxyphenyl 2,2,3,3,...	360	C14H11F7O3	1000366-95-1	14		
2	Benzaldehyde, 4-(methylthio)-	152	C8H8OS	003446-89-7	14		
3	2,4-Dinitro-11-phenyl-5H-dibenzo...	360	C19H12N4O4	071354-26-2	12		
4	1,3-Dithiane, 4,5-dimethyl-2-(4-...	254	C13H18OS2	1000197-88-6	10		
5	Hexafluoro-2,2-bis-(3,4-dimethyl...	360	C19H18F6	065294-20-4	9		



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.181	5.3	ng	75220	1	6.857	284045	20.0
Nonahexacontano...	13.827	3.2	ng	61714	5	14.033	390686	20.0
unknown17.07	17.074	6.5	ng	100728	6	15.515	308491	20.0