

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061121\
 Data File : BF124259.D
 Acq On : 11 Jun 2021 14:11
 Operator : JU/CG
 Sample : M2638-02
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ND-1

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: BF124259.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	11	14	19	rVB2	15147	19266	1.61%	0.228%
2	5.051	500	504	511	rVB2	46280	56231	4.71%	0.664%
3	5.469	571	575	585	rVB	996616	841952	70.50%	9.945%
4	6.487	743	748	753	rBV	832576	840045	70.34%	9.923%
5	6.839	805	808	811	rBV	285775	211796	17.73%	2.502%
6	7.404	899	904	907	rBV	675308	569428	47.68%	6.726%
7	8.028	1006	1010	1018	rBV2	16565	22390	1.87%	0.264%
8	8.122	1023	1026	1030	rBV	350106	278869	23.35%	3.294%
9	9.198	1205	1209	1212	rBV	1311420	1087107	91.03%	12.841%
10	9.880	1321	1325	1328	rBV	453798	354342	29.67%	4.185%
11	10.669	1455	1459	1463	rBV	903119	822584	68.88%	9.716%
12	11.369	1574	1578	1581	rBV	470000	371914	31.14%	4.393%
13	11.892	1662	1667	1672	rBV	96207	95101	7.96%	1.123%
14	12.580	1780	1784	1794	rBV	83243	83420	6.99%	0.985%
15	12.680	1797	1801	1806	rVB2	28412	30458	2.55%	0.360%
16	12.810	1818	1823	1828	rVB	87007	86397	7.23%	1.021%
17	12.957	1843	1848	1851	rBV	1387870	1194254	100.00%	14.106%
18	13.139	1873	1879	1882	rVB3	11486	24444	2.05%	0.289%
19	13.245	1894	1897	1903	rVB5	16037	19330	1.62%	0.228%
20	13.757	1979	1984	1987	rBV5	10503	15121	1.27%	0.179%
21	13.798	1987	1991	1995	rBV3	25257	48684	4.08%	0.575%
22	13.868	1995	2003	2010	rVB5	116838	227391	19.04%	2.686%
23	13.986	2017	2023	2024	rBV4	39579	52302	4.38%	0.618%
24	14.015	2024	2028	2030	rVV	317694	341288	28.58%	4.031%
25	14.039	2030	2032	2034	rVB	40010	30968	2.59%	0.366%
26	14.168	2050	2054	2057	rBV4	10771	15555	1.30%	0.184%
27	14.368	2086	2088	2091	rBV3	12832	17415	1.46%	0.206%
28	14.445	2097	2101	2103	rBV5	9890	14392	1.21%	0.170%
29	14.527	2111	2115	2116	rBV3	12687	14298	1.20%	0.169%
30	14.862	2168	2172	2175	rBV	58986	62344	5.22%	0.736%
31	15.057	2201	2205	2213	rBV3	57084	104975	8.79%	1.240%
32	15.127	2214	2217	2221	rVB4	18784	18235	1.53%	0.215%
33	15.168	2221	2224	2226	rBV4	17255	20316	1.70%	0.240%
34	15.362	2254	2257	2263	rVB2	28392	36095	3.02%	0.426%
35	15.427	2265	2268	2274	rVB2	38777	46780	3.92%	0.553%
36	15.492	2274	2279	2284	rBV	212630	261085	21.86%	3.084%

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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

37	15.645	2300	2305	2306	rBV4	13486	17034	1.43%	0.201%
38	15.939	2353	2355	2361	rVB5	17945	23427	1.96%	0.277%
39	16.974	2526	2531	2534	rBV5	26895	43756	3.66%	0.517%
40	17.427	2601	2608	2613	rVB4	19867	45215	3.79%	0.534%

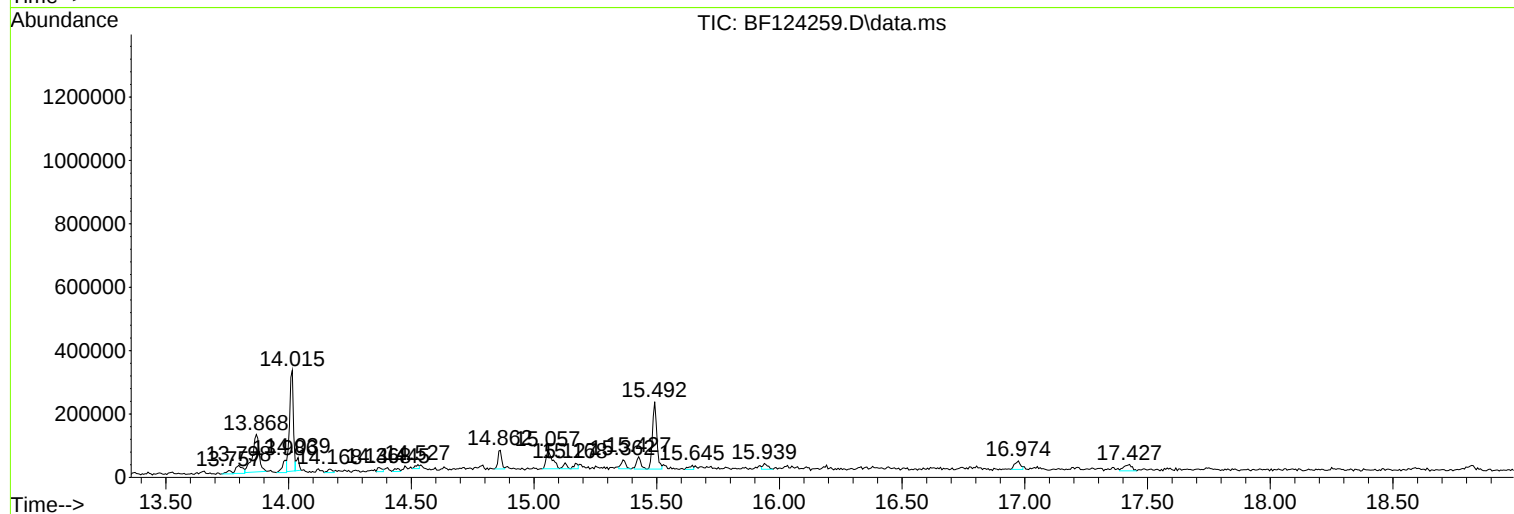
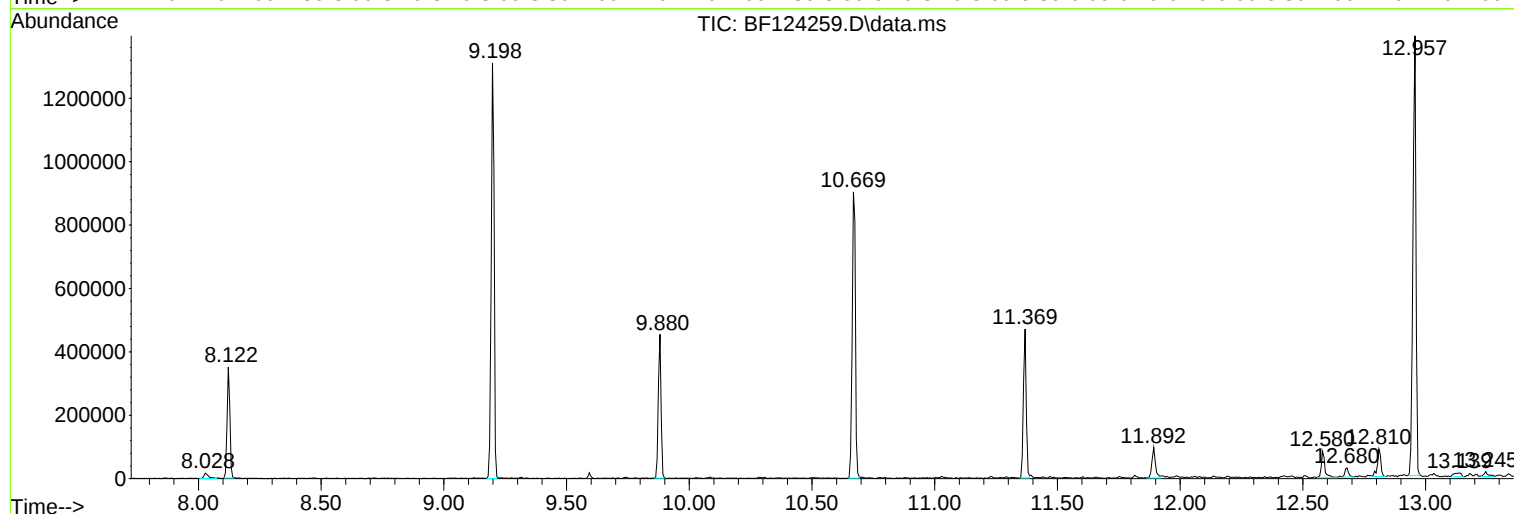
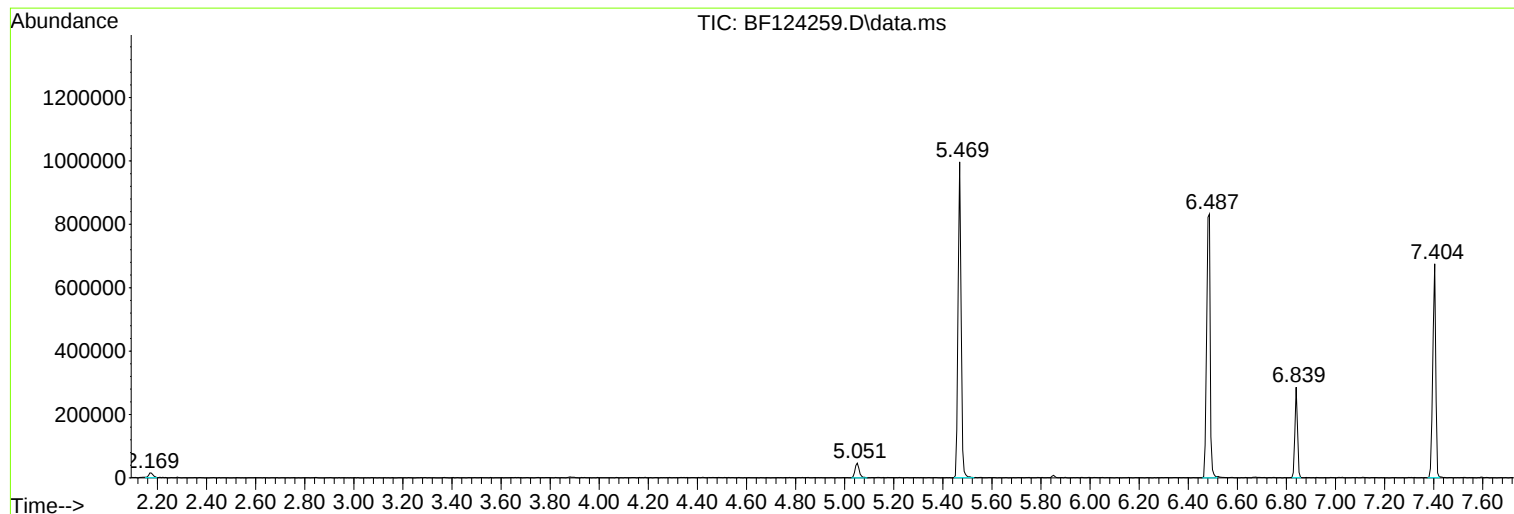
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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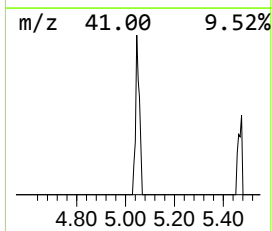
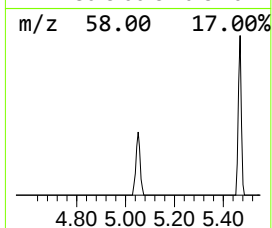
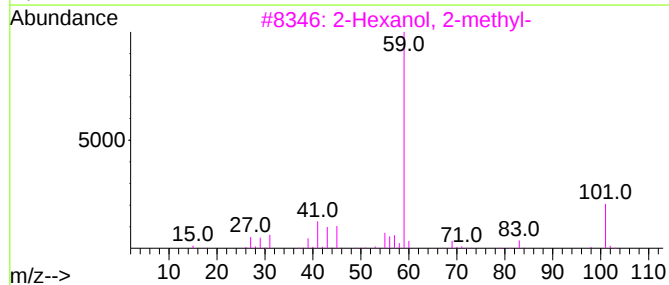
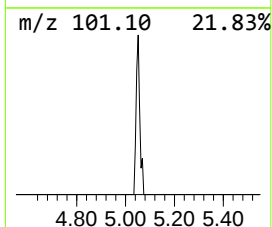
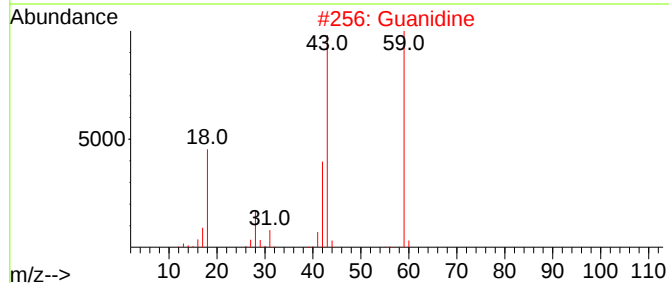
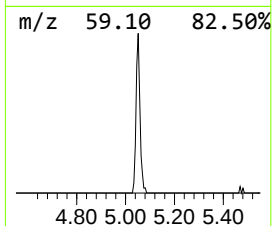
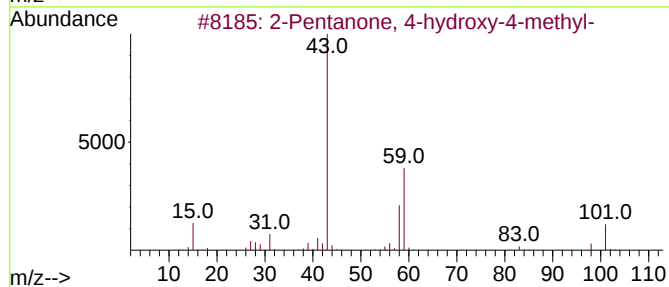
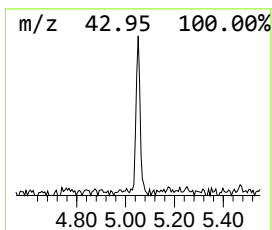
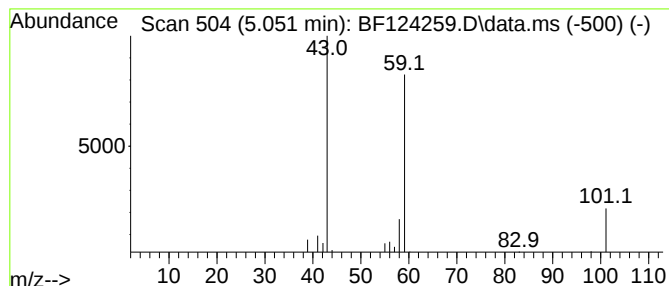
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	5.31 ng	56231	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Guanidine	59	CH5N3	000113-00-8	50		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	50		
4	3-Heptanol	116	C7H16O	000589-82-2	36		
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	33		



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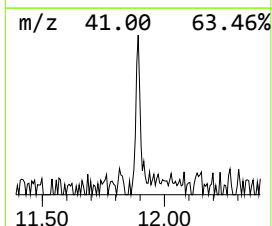
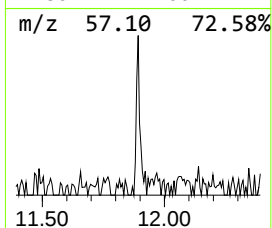
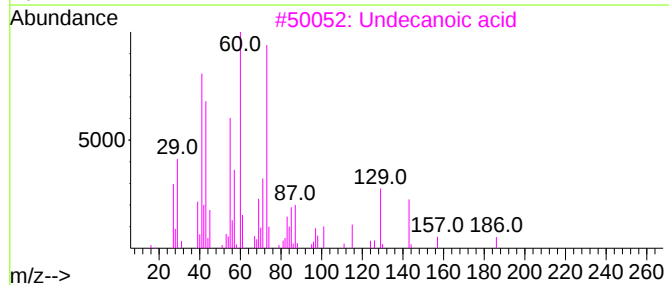
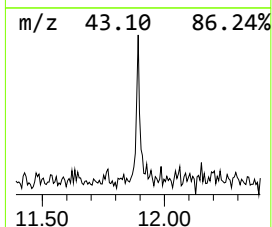
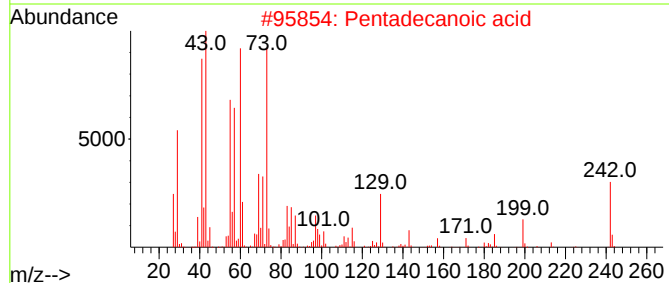
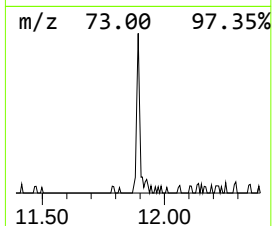
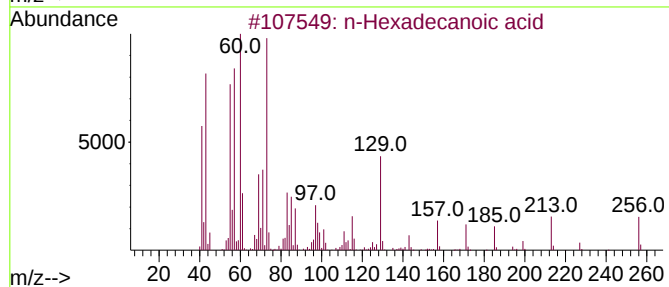
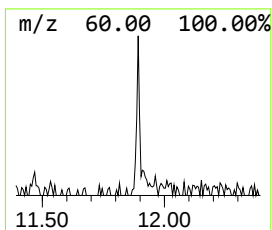
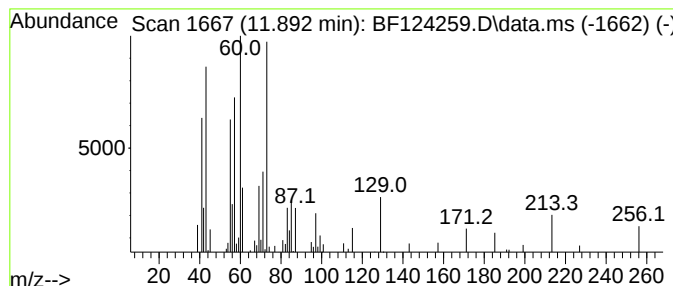
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	5.11 ng	95101	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3			Undecanoic acid	186	C11H22O2	000112-37-8	72
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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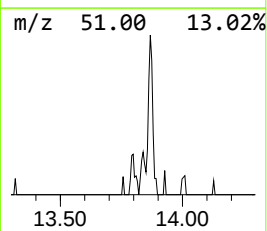
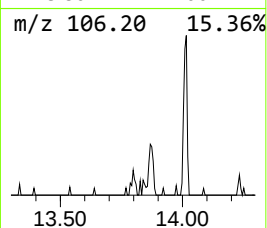
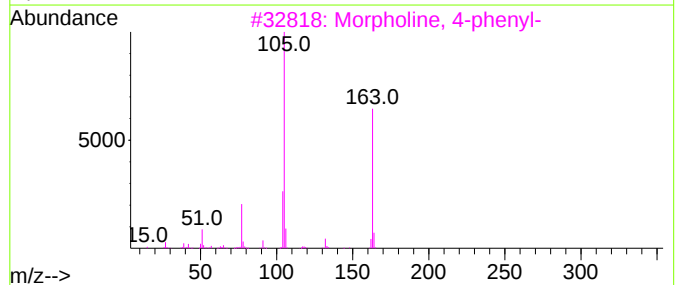
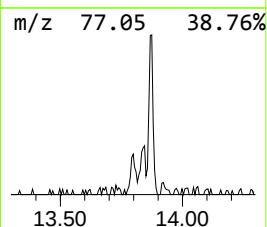
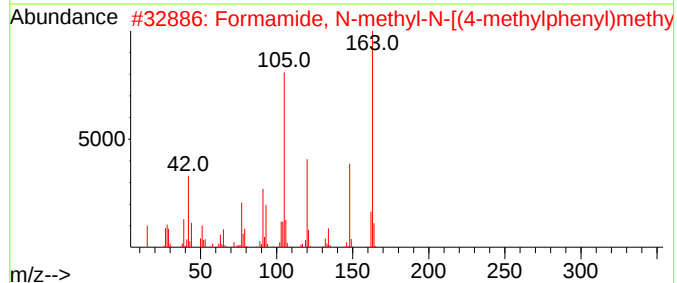
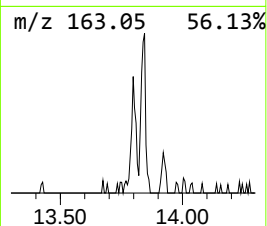
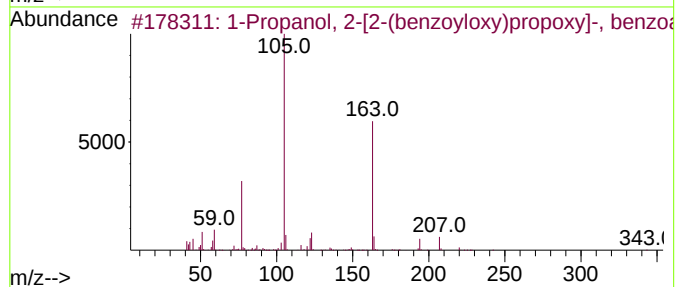
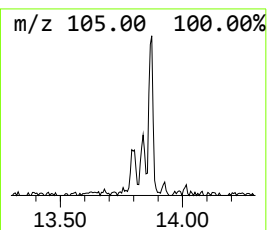
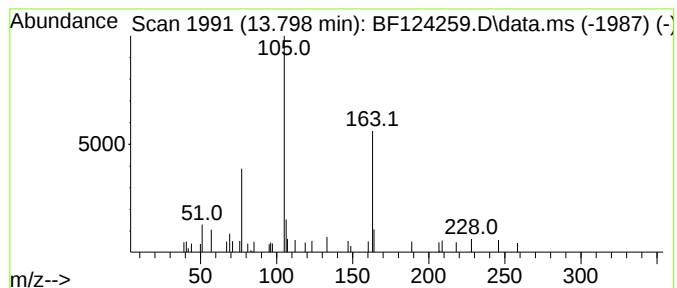
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Propanol, 2-[2-(benzoylox... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	2.85 ng	48684	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	50		
2	Formamide, N-methyl-N-[(4-methyl...	163	C10H13NO	054410-77-4	47		
3	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	47		
4	Benzoic acid, 1-methylethyl ester	164	C10H12O2	000939-48-0	43		
5	3-Nitro-1-(2-oxo-2-phenyl-ethyl)...	258	C13H10N2O4	1000275-72-5	38		



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Instrument :
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ClientSampled :
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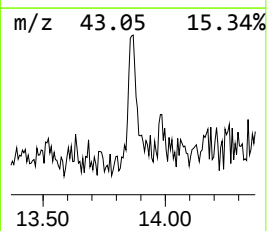
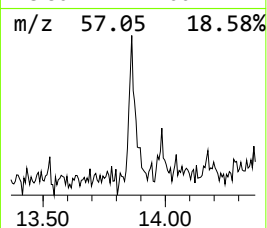
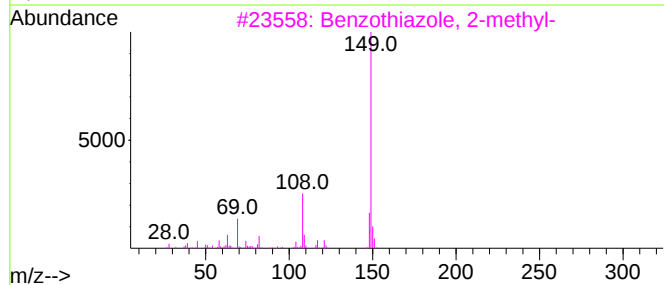
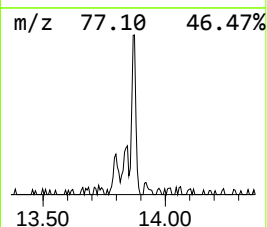
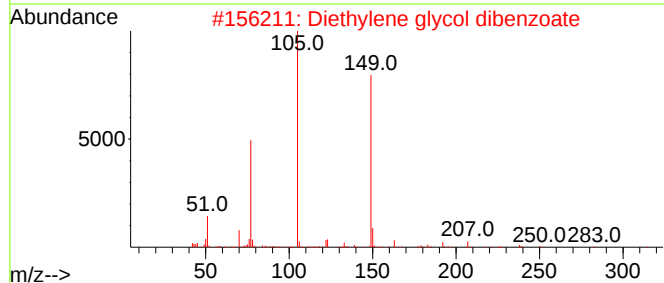
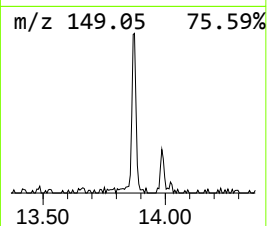
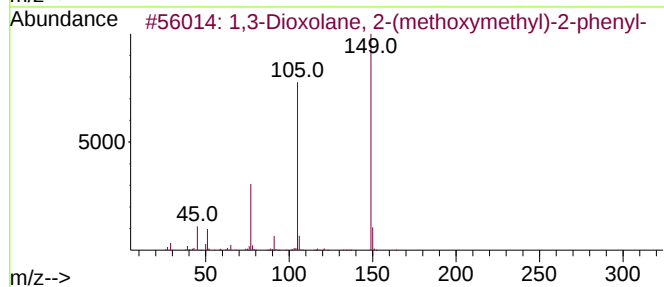
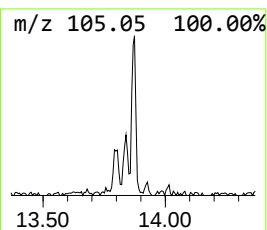
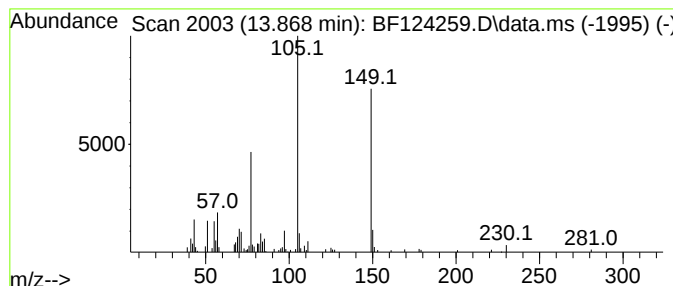
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	13.33 ng	227391	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	72
2			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
3			Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	38
4			Benzoic acid, ethyl ester	150	C9H10O2	000093-89-0	27
5			Benzoic acid 2-(4-chloro-phenyl)...	370	C21H19ClO4	1000274-89-7	27



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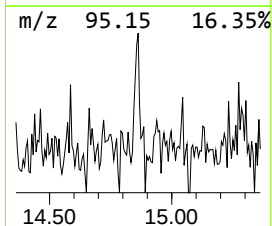
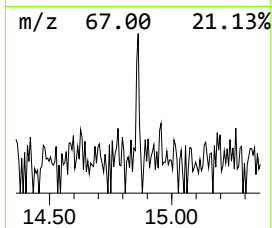
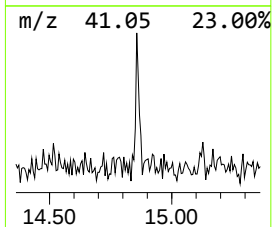
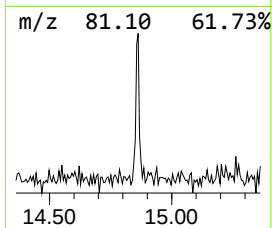
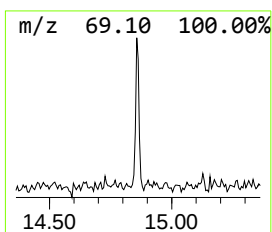
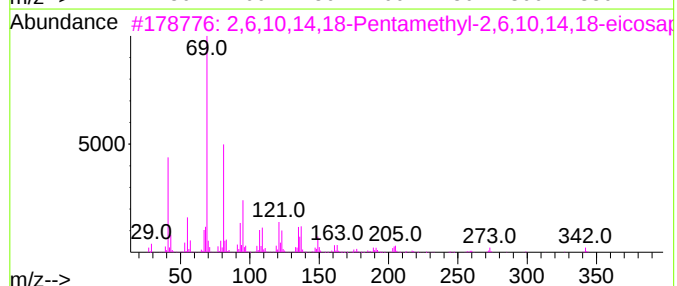
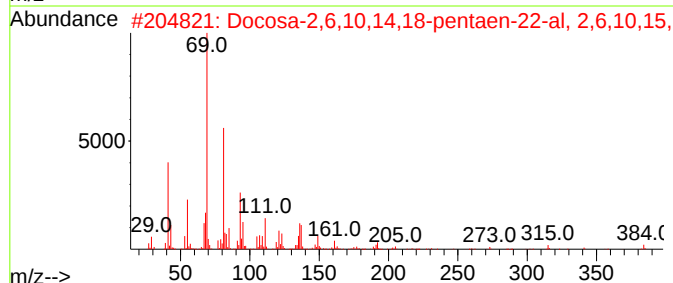
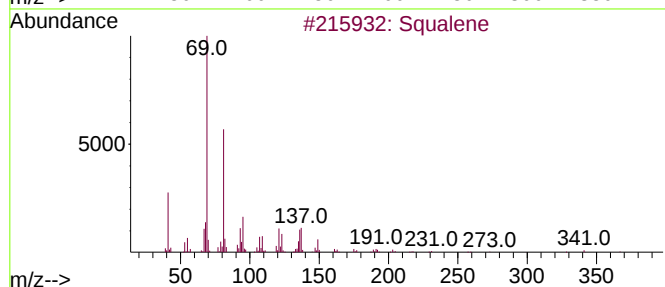
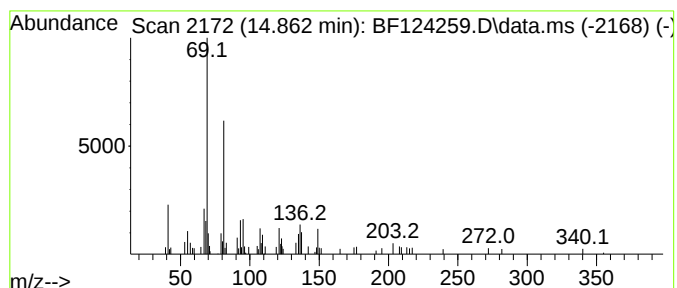
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.862	4.78 ng	62344	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
3			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	78
4			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
5			3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061121\
Data File : BF124259.D
Acq On : 11 Jun 2021 14:11
Operator : JU/CG
Sample : M2638-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ND-1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.051	5.3	ng	56231	1	6.839	211796	20.0
n-Hexadecanoic ...	11.892	5.1	ng	95101	4	11.368	371914	20.0
1-Propanol, 2-[...	13.798	2.9	ng	48684	5	14.015	341288	20.0
1,3-Dioxolane, ...	13.868	13.3	ng	227391	5	14.015	341288	20.0
Squalene	14.862	4.8	ng	62344	6	15.492	261085	20.0