

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012622\
 Data File : BF126702.D
 Acq On : 26 Jan 2022 22:17
 Operator : CG/JU
 Sample : N1266-06
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-08-(5-6)

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-BF011822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126702.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.298	28	36	42	rVB	492004	633340	14.85%	2.012%
2	4.098	338	342	347	rVB	40952	48010	1.13%	0.153%
3	5.198	525	529	535	rVB	46985	54049	1.27%	0.172%
4	5.575	588	593	596	rBV	4318773	4252260	99.72%	13.510%
5	6.569	756	762	765	rBV	3971832	4264120	100.00%	13.548%
6	6.957	824	828	831	rVB	1018739	892773	20.94%	2.837%
7	7.516	918	923	926	rBV	2998831	2785768	65.33%	8.851%
8	8.127	1024	1027	1033	rBV	44562	48011	1.13%	0.153%
9	8.239	1041	1046	1049	rBV	1432782	1330644	31.21%	4.228%
10	9.316	1224	1229	1232	rBV	4092294	3709598	87.00%	11.786%
11	9.998	1341	1345	1348	rVB	1291137	1114744	26.14%	3.542%
12	10.545	1435	1438	1441	rVB	47103	43641	1.02%	0.139%
13	10.786	1475	1479	1482	rBV	3024267	2601309	61.00%	8.265%
14	11.380	1575	1580	1585	rVB3	61035	76517	1.79%	0.243%
15	11.486	1594	1598	1601	rBV	1788759	1656154	38.84%	5.262%
16	11.510	1601	1602	1606	rVV	639851	390725	9.16%	1.241%
17	11.563	1606	1611	1614	rVB	137438	123263	2.89%	0.392%
18	11.986	1680	1683	1686	rBV	129877	139359	3.27%	0.443%
19	12.015	1686	1688	1693	rVB	153309	130800	3.07%	0.416%
20	12.098	1699	1702	1705	rBV2	140780	174464	4.09%	0.554%
21	12.121	1705	1706	1710	rVB	106129	78710	1.85%	0.250%
22	12.539	1774	1777	1779	rBV	66549	65251	1.53%	0.207%
23	12.580	1782	1784	1789	rVB4	63454	70895	1.66%	0.225%
24	12.704	1802	1805	1808	rBV	249718	199828	4.69%	0.635%
25	12.933	1838	1844	1851	rBV	317301	319041	7.48%	1.014%
26	13.080	1864	1869	1872	rBV	3745831	3497257	82.02%	11.111%
27	13.151	1878	1881	1888	rVB2	30520	45893	1.08%	0.146%
28	13.262	1897	1900	1903	rVB	46167	45211	1.06%	0.144%
29	13.980	2016	2022	2024	rBV3	85364	130964	3.07%	0.416%
30	14.133	2040	2048	2051	rBV	1062135	1040453	24.40%	3.306%
31	14.162	2051	2053	2058	rVB	92391	89060	2.09%	0.283%
32	15.004	2191	2196	2200	rBV2	106442	123458	2.90%	0.392%
33	15.204	2226	2230	2234	rBV2	38506	69286	1.62%	0.220%
34	15.521	2280	2284	2289	rVB	44921	58758	1.38%	0.187%
35	15.586	2291	2295	2301	rVB	56826	78111	1.83%	0.248%
36	15.656	2301	2307	2318	rBV2	799225	1045242	24.51%	3.321%

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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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.203	2565	2570	2580	rVB4	18756	47312	1.11%	0.150%
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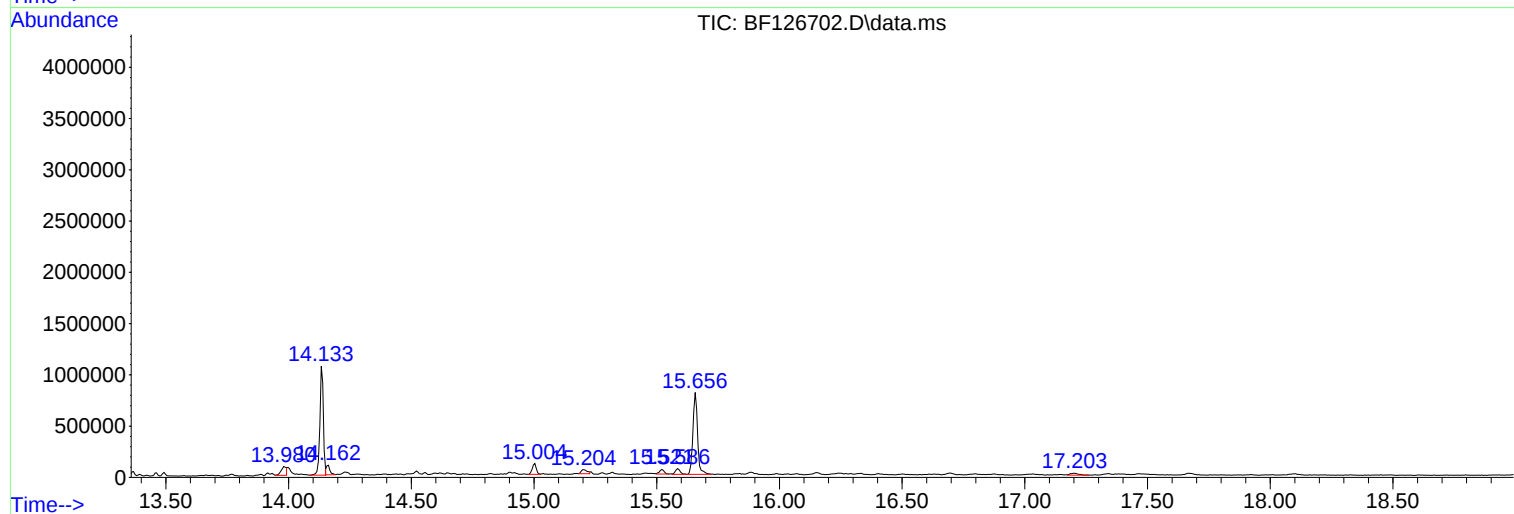
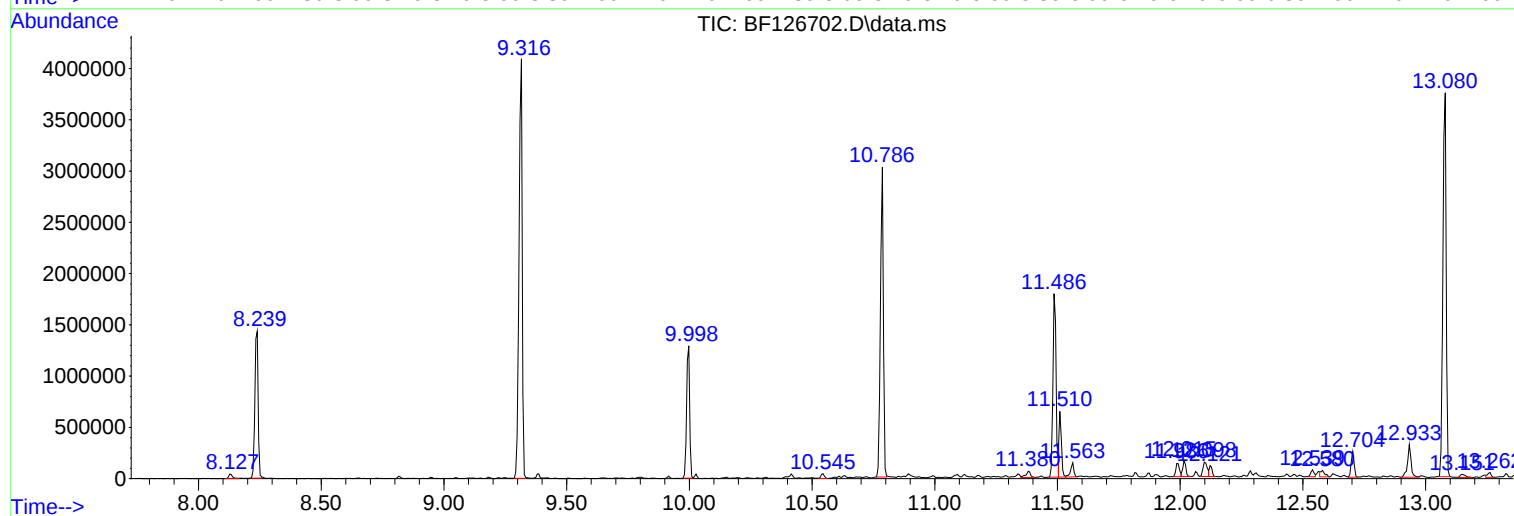
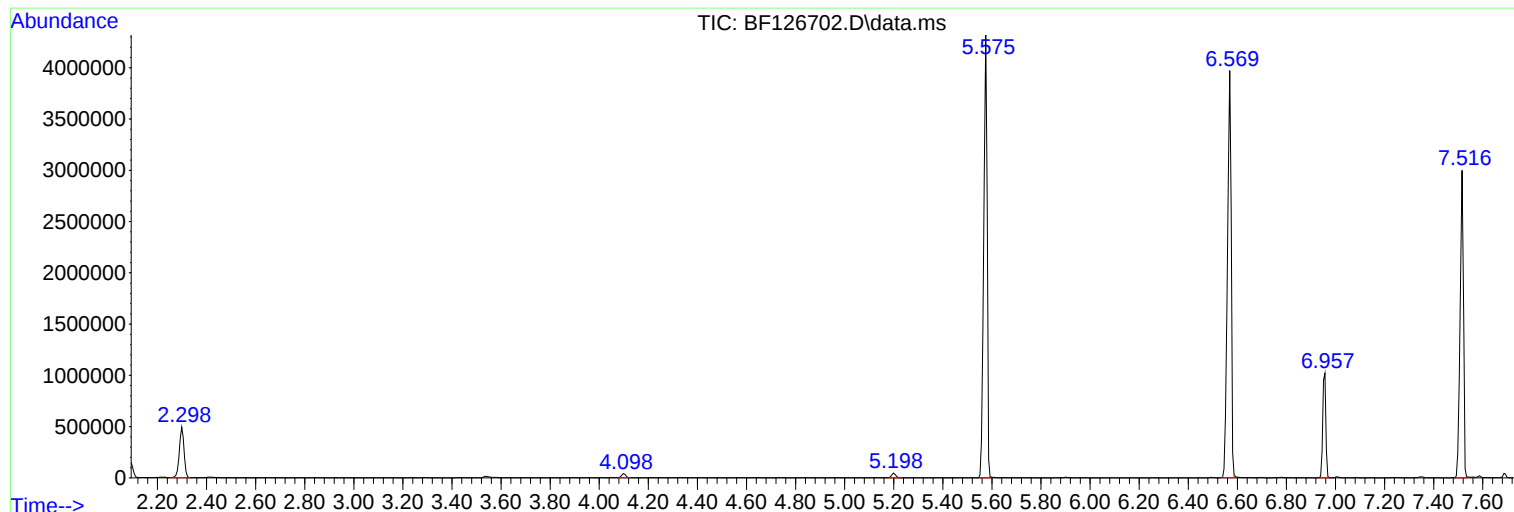
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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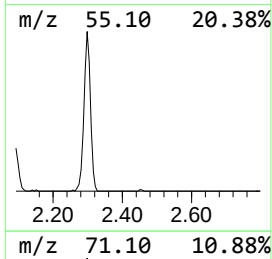
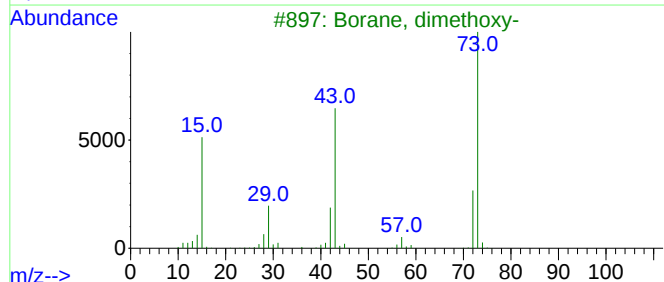
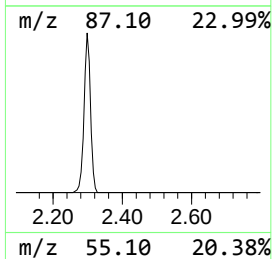
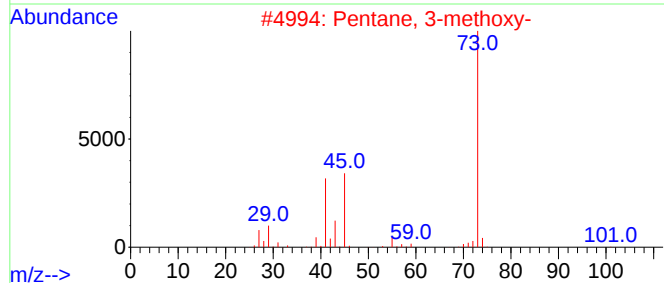
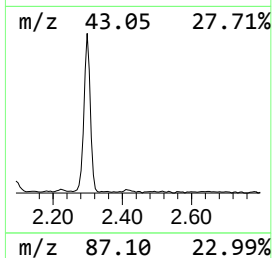
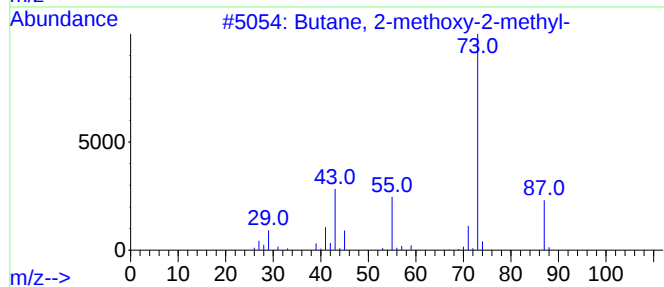
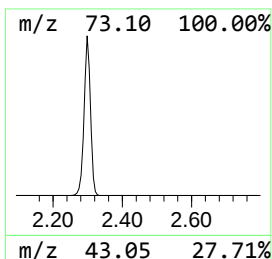
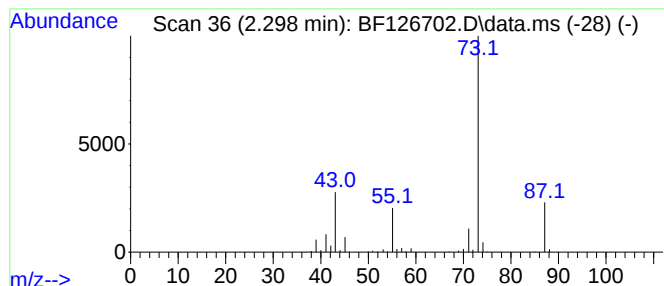
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.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.
2.298	14.19 ng	633340	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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RB-08-(5-6)

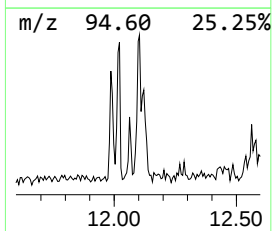
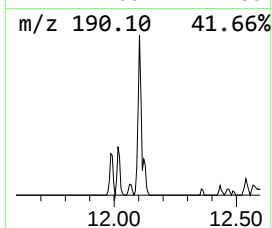
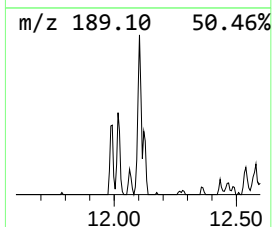
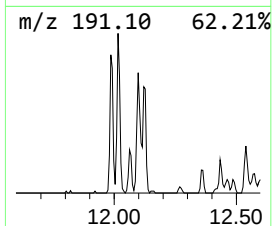
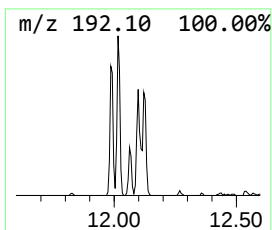
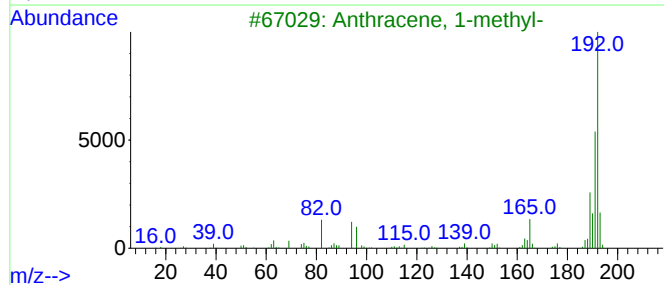
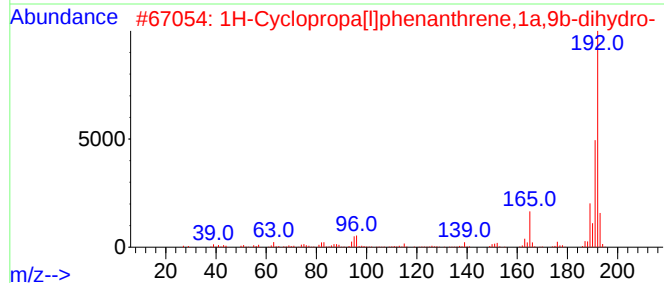
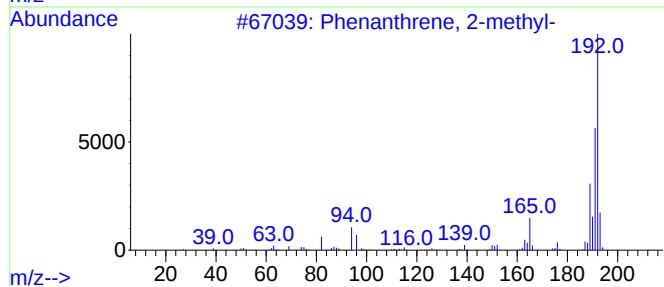
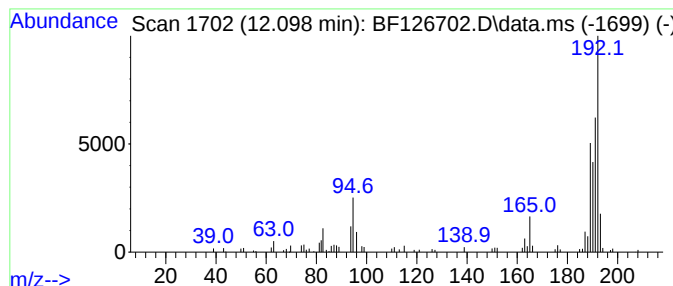
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Phenanthrene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.098	2.11 ng	174464	Phenanthrene-d10	11.486

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
2		1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	91
3		Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
4		Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
5		5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	90



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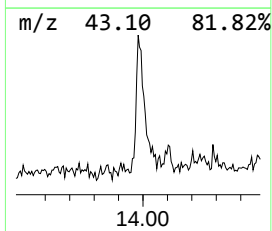
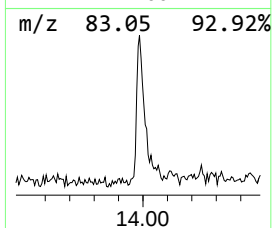
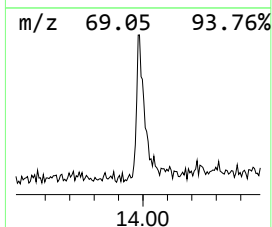
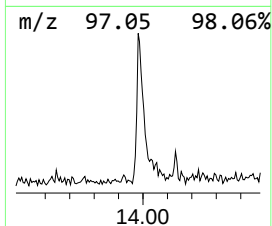
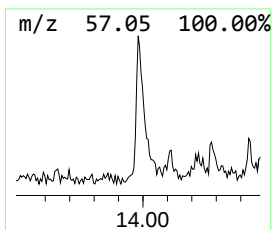
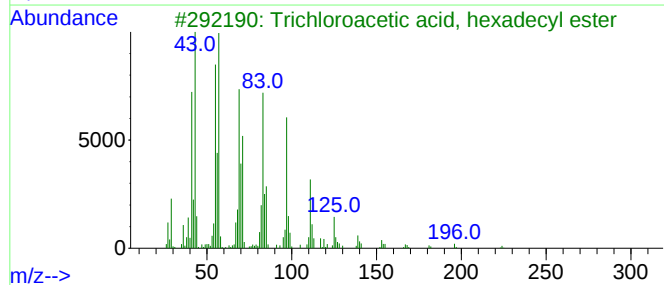
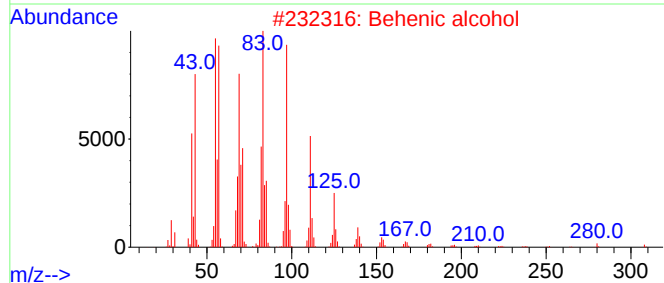
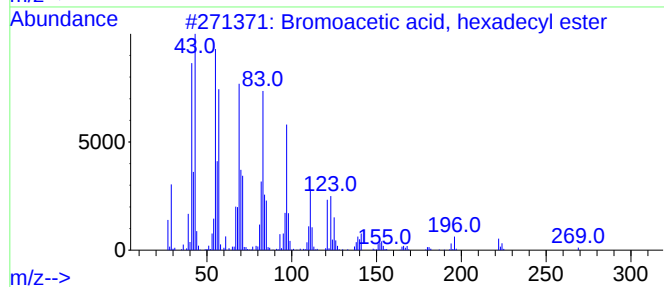
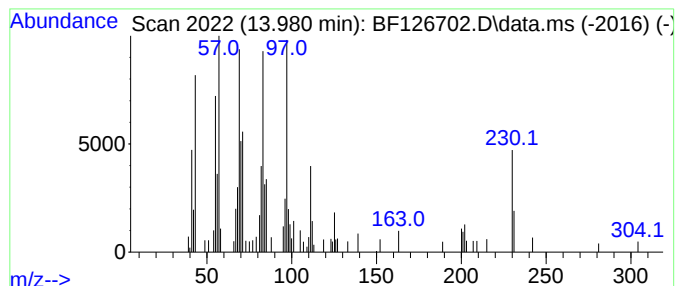
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Bromoacetic acid, hexadecyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	2.52 ng	130964	Chrysene-d12	14.133

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
2			Behenic alcohol	326	C22H46O	000661-19-8	87
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	81
5			1-Tricosene	322	C23H46	018835-32-0	81



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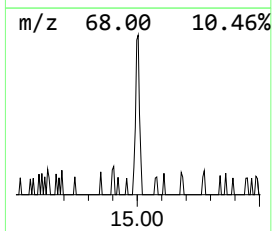
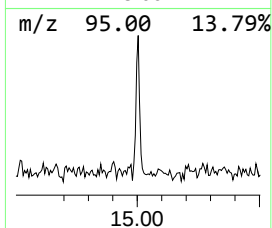
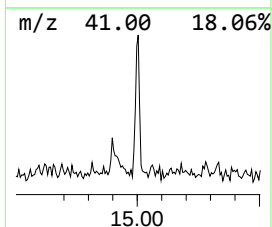
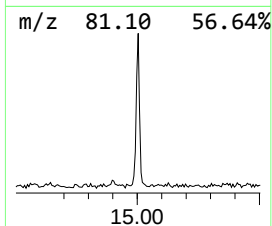
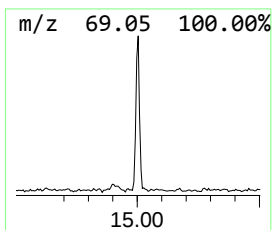
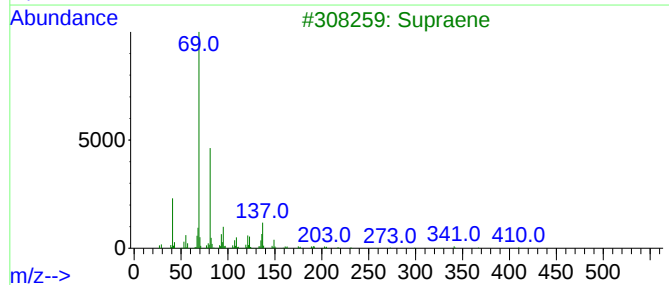
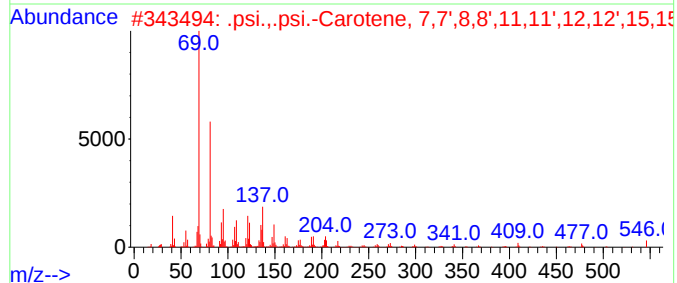
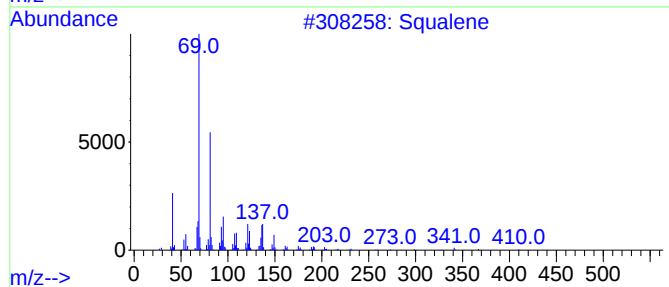
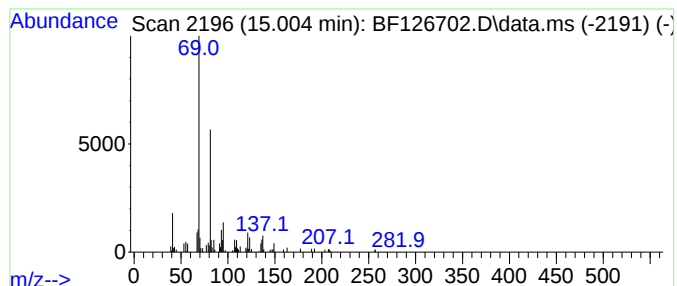
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.004	2.36 ng	123458	Perylene-d12	15.656

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
3			Supraene	410	C30H50	007683-64-9	80
4			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64
5			trans-Farnesol	222	C15H26O	000106-28-5	64



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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...	2.298	14.2	ng	633340	1	6.957	892773	20.0
Phenanthrene, 2...	12.098	2.1	ng	174464	4	11.486	1656150	20.0
Bromoacetic aci...	13.980	2.5	ng	130964	5	14.133	1040450	20.0
Squalene	15.004	2.4	ng	123458	6	15.656	1045240	20.0