

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042123\
 Data File : BM039571.D
 Acq On : 22 Apr 2023 03:06
 Operator : CG/JU
 Sample : 02426-01 2X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 EO-3-041923

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_M\Methods\8270-BM041723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039571.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.919	315	320	326	rBV	36437	55593	1.84%	0.195%
2	5.402	396	402	421	rBV	1048335	1727640	57.10%	6.059%
3	7.019	669	677	689	rBV	929043	1666287	55.07%	5.844%
4	7.131	691	696	705	rVB	33563	73933	2.44%	0.259%
5	7.825	806	814	829	rBV	710809	1146399	37.89%	4.021%
6	8.995	1007	1013	1032	rBV	558387	1060453	35.05%	3.719%
7	10.637	1280	1292	1299	rBV	845777	1529968	50.56%	5.366%
8	12.048	1523	1532	1538	rBV3	36766	75432	2.49%	0.265%
9	12.301	1572	1575	1583	rVB	30798	46639	1.54%	0.164%
10	12.448	1592	1600	1605	rBV2	23044	62222	2.06%	0.218%
11	12.525	1609	1613	1622	rVB2	37484	85491	2.83%	0.300%
12	13.007	1691	1695	1702	rVB	41973	68058	2.25%	0.239%
13	13.101	1705	1711	1721	rBV	1594522	2407079	79.55%	8.442%
14	13.295	1741	1744	1753	rVB2	43502	75658	2.50%	0.265%
15	13.742	1814	1820	1825	rBV2	142242	220443	7.29%	0.773%
16	13.801	1825	1830	1836	rVV3	42283	92871	3.07%	0.326%
17	14.207	1895	1899	1910	rVB	46060	83617	2.76%	0.293%
18	14.372	1923	1927	1934	rBV	53655	73672	2.43%	0.258%
19	14.483	1940	1946	1953	rBV	1207217	1816102	60.02%	6.370%
20	14.548	1953	1957	1962	rVB	120098	168466	5.57%	0.591%
21	14.883	2010	2014	2025	rVB2	58636	98373	3.25%	0.345%
22	15.324	2086	2089	2093	rVB	44202	53820	1.78%	0.189%
23	15.536	2120	2125	2137	rBV	130149	214452	7.09%	0.752%
24	15.766	2161	2164	2170	rVB3	83245	120389	3.98%	0.422%
25	15.848	2171	2178	2185	rBV2	192428	313630	10.37%	1.100%
26	15.983	2195	2201	2208	rBV	1149160	1726681	57.07%	6.056%
27	16.195	2233	2237	2238	rBV	52677	67651	2.24%	0.237%
28	16.983	2369	2371	2375	rVB	54518	56507	1.87%	0.198%
29	17.242	2409	2415	2418	rBV	1374497	2047766	67.68%	7.182%
30	17.283	2418	2422	2431	rVV	1018279	1489710	49.23%	5.225%
31	17.371	2433	2437	2442	rVV	270767	375558	12.41%	1.317%
32	18.136	2561	2567	2570	rBV2	342979	633325	20.93%	2.221%
33	18.248	2583	2586	2591	rVB	102270	135755	4.49%	0.476%
34	18.312	2593	2597	2601	rBV2	207510	334367	11.05%	1.173%
35	19.301	2761	2765	2774	rBV	1599225	2296187	75.89%	8.053%
36	19.636	2819	2822	2823	rBV2	278392	300745	9.94%	1.055%

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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_M\Methods\8270-BM041723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.665	2824	2827	2836	rVB2	1242342	2042751	67.51%	7.164%
38	19.865	2857	2861	2868	rBV	2477212	3025810	100.00%	10.612%
39	20.512	2968	2971	2975	rBV2	529030	642848	21.25%	2.255%

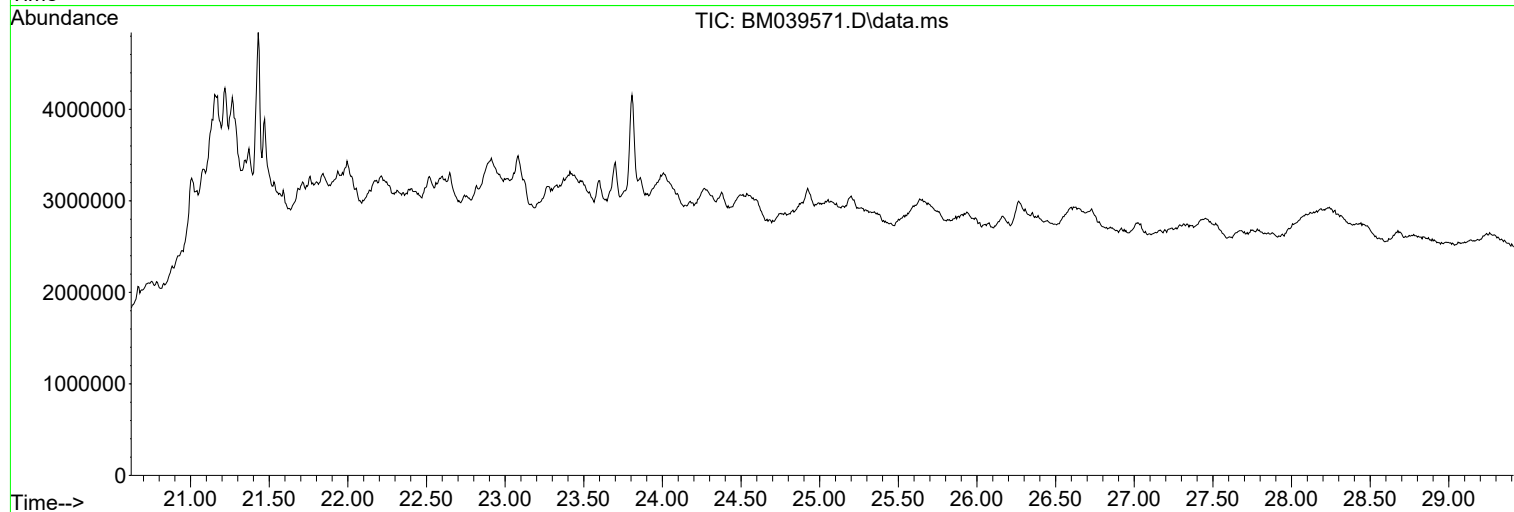
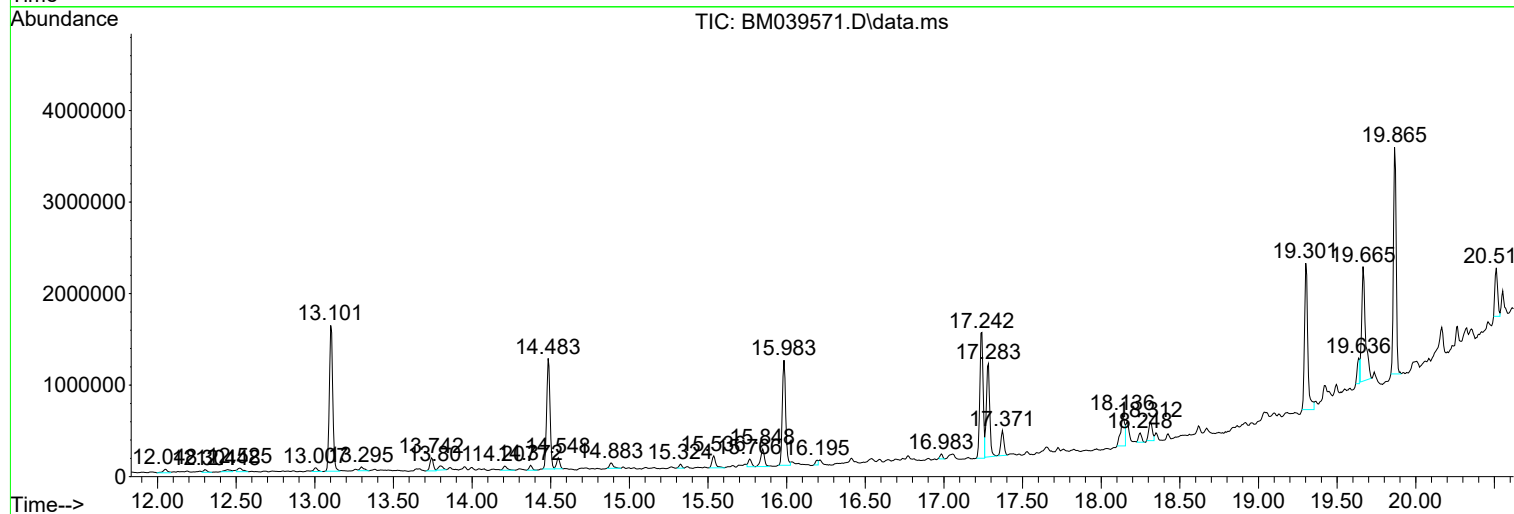
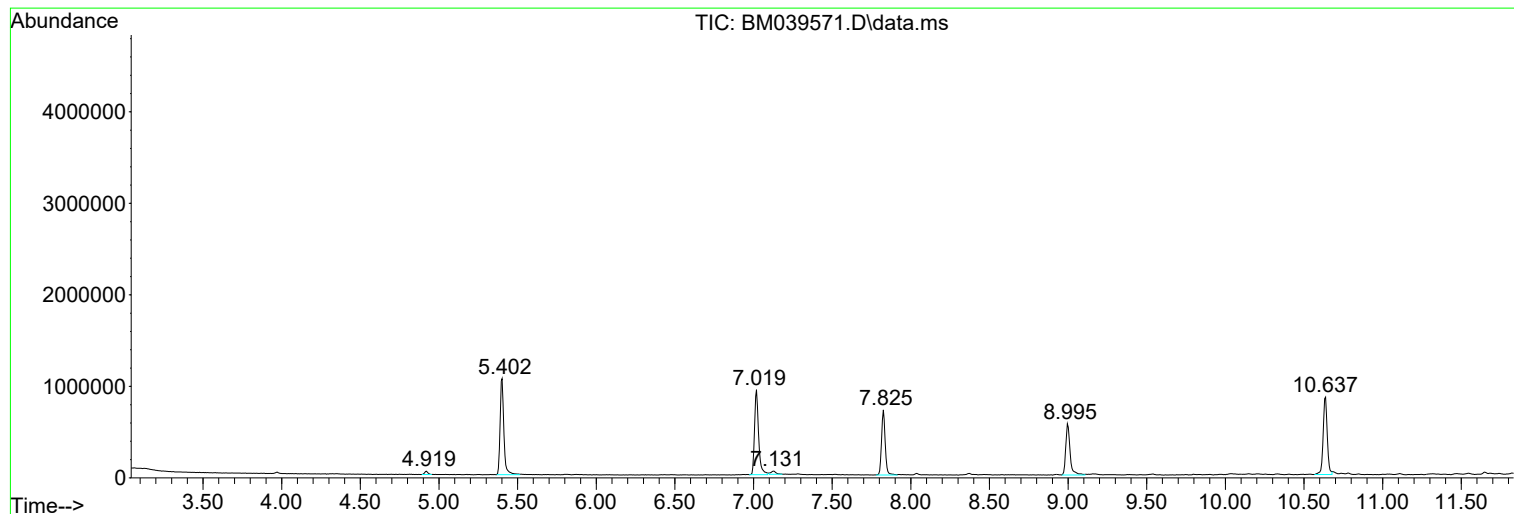
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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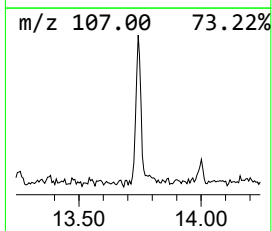
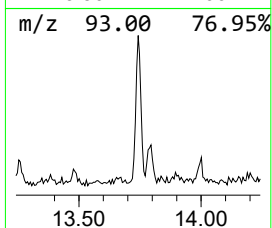
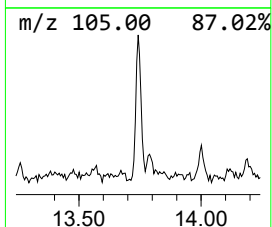
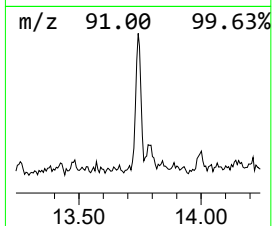
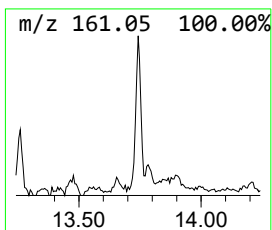
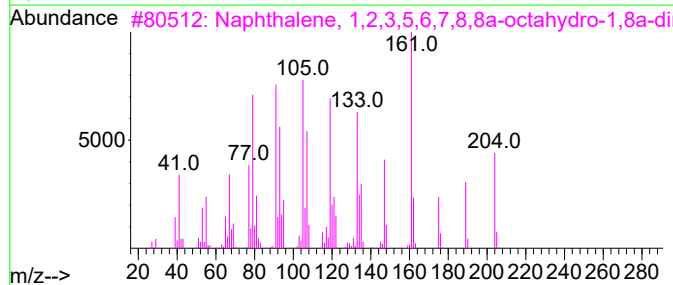
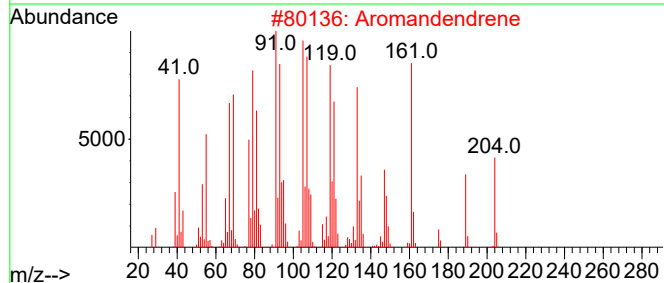
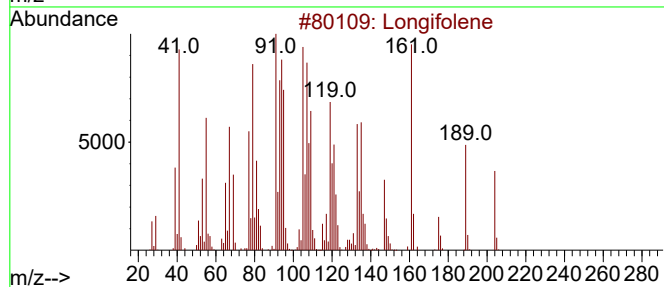
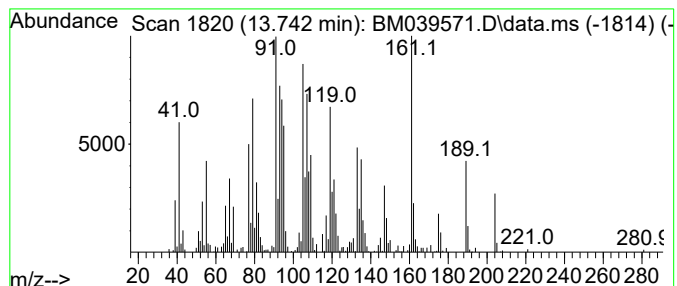
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Longifolene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.742	2.43 ng	220443	Acenaphthene-d10	14.483

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Longifolene	204	C15H24	000475-20-7	99
2			Aromandendrene	204	C15H24	000489-39-4	95
3			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	95
4			1,2,4-Methenoazulene, decahydro-...	204	C15H24	001137-12-8	95
5			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	010219-75-7	91



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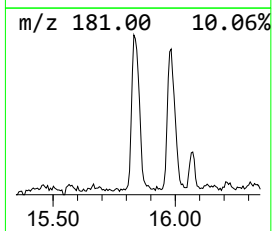
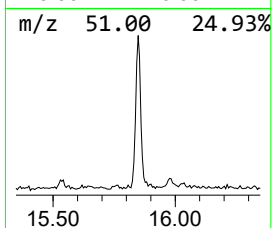
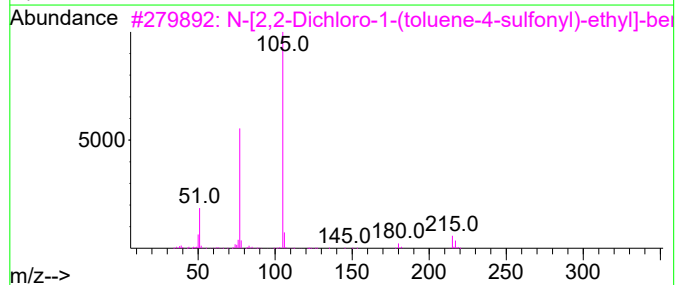
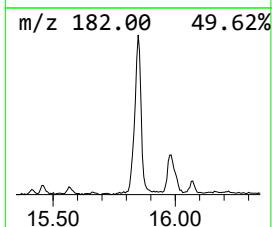
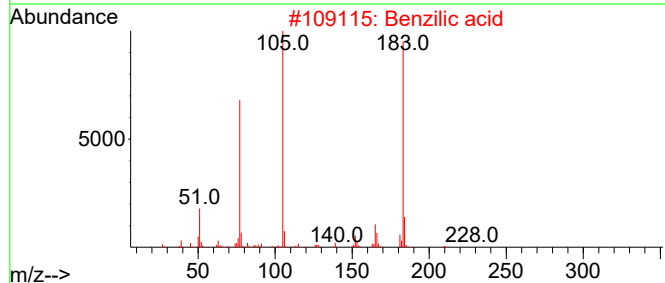
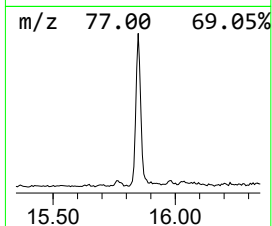
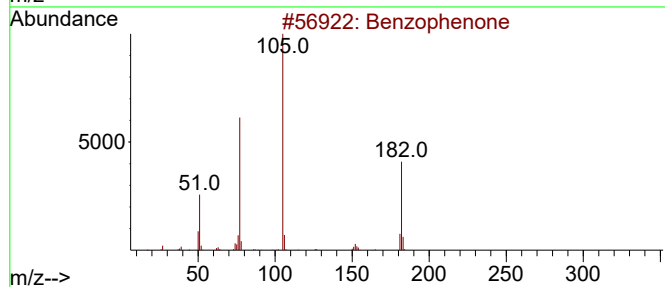
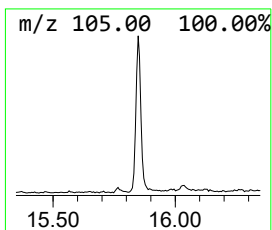
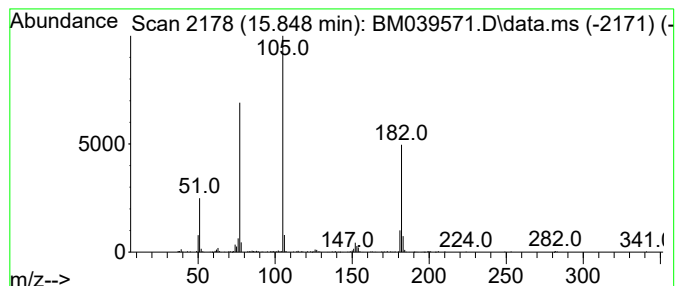
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM041723.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.848	3.45 ng	313630	Acenaphthene-d10	14.483

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzilic acid	228	C14H12O3	000076-93-7	47
3			N-[2,2-Dichloro-1-(toluene-4-sul...	371	C16H15Cl2NO3S	136800-77-6	47
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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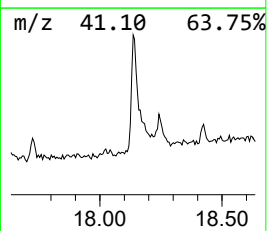
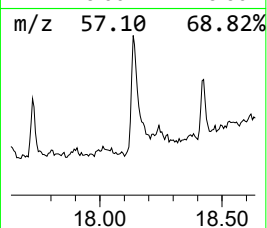
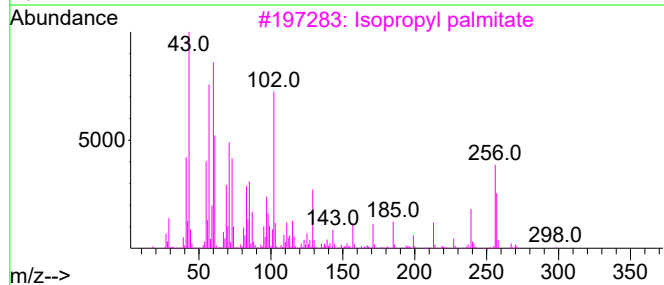
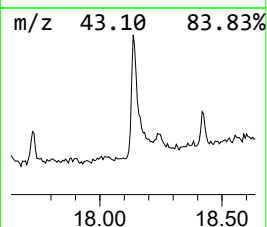
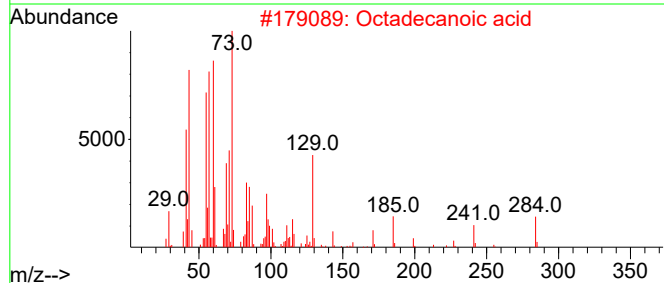
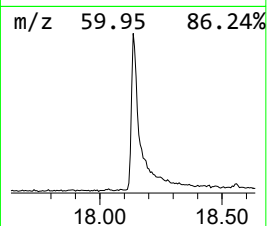
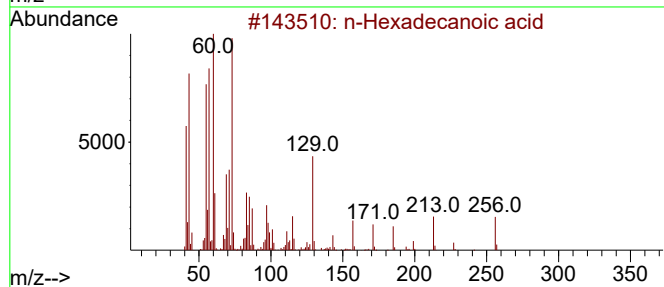
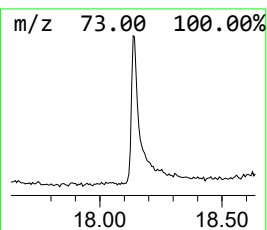
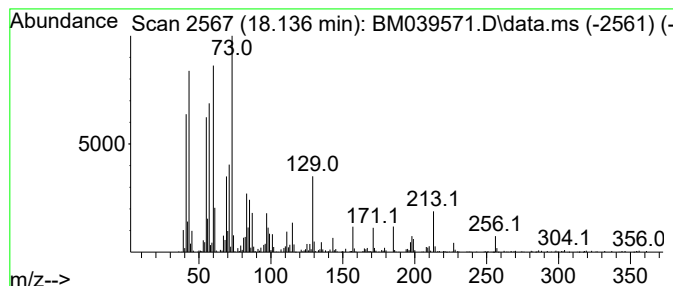
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.136	6.19 ng	633325	Phenanthrene-d10	17.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	90
3			Isopropyl palmitate	298	C19H38O2	000142-91-6	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	87



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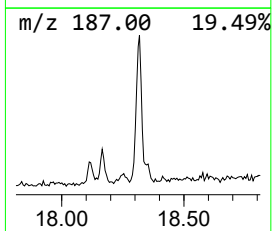
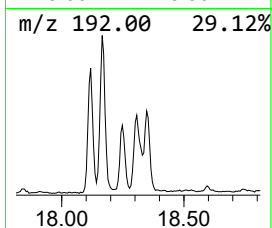
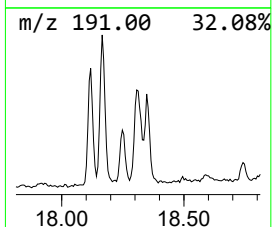
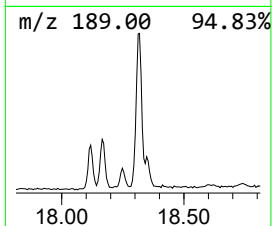
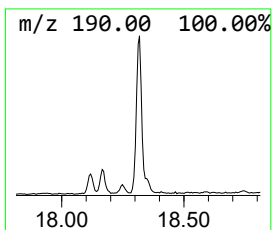
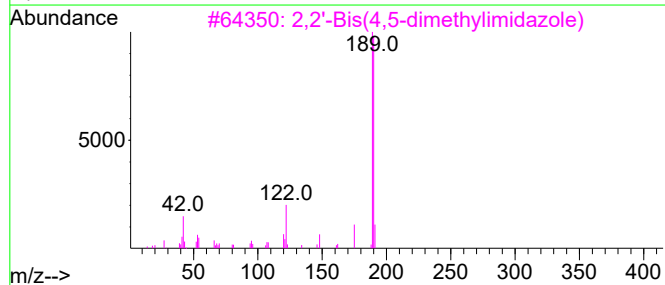
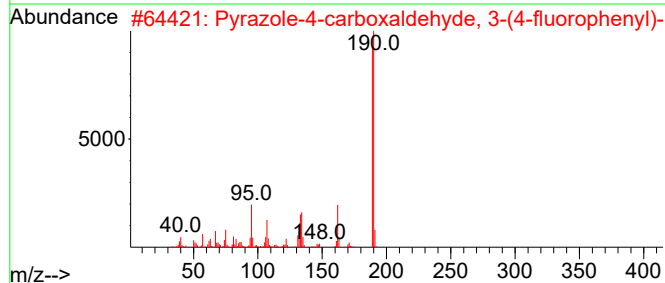
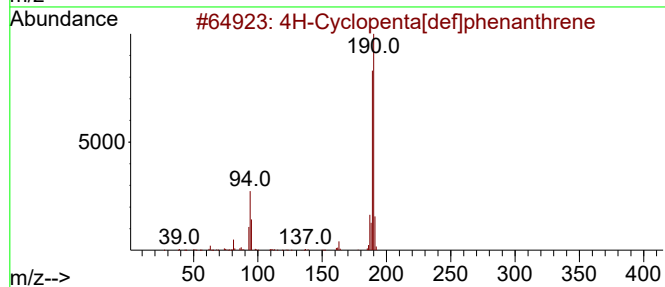
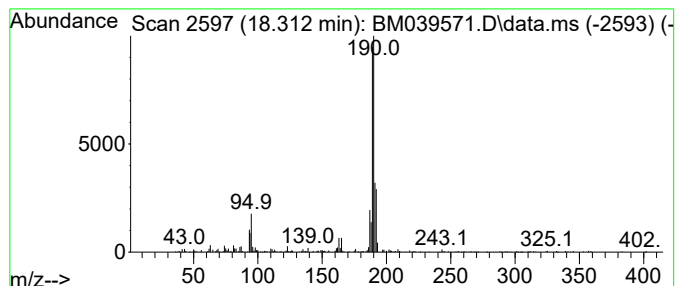
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.313	3.27 ng	334367	Phenanthrene-d10	17.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	91
2			Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	58
3			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	52
4			Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
5			2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50



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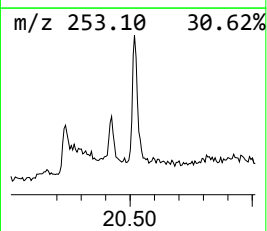
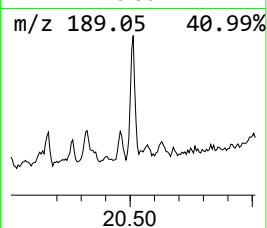
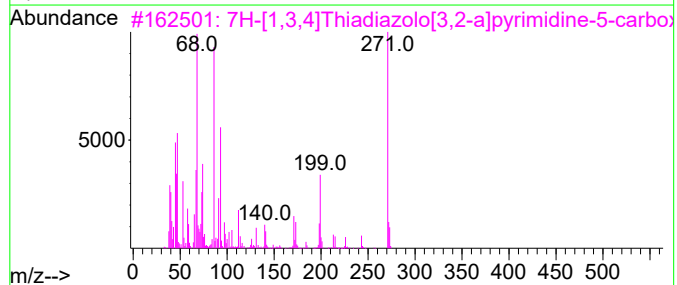
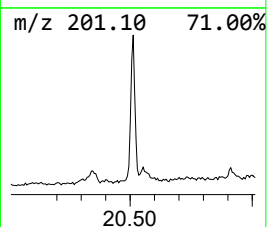
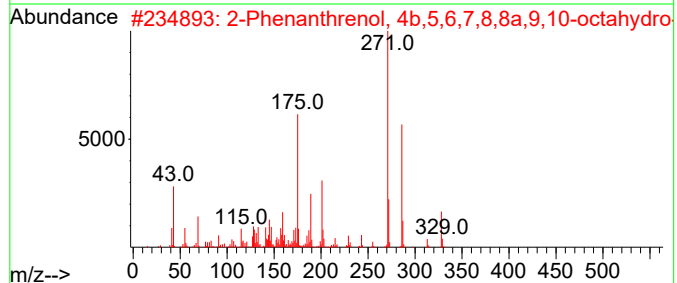
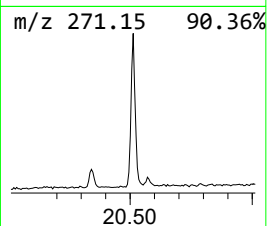
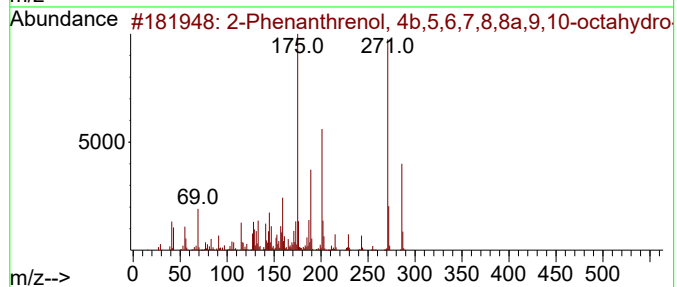
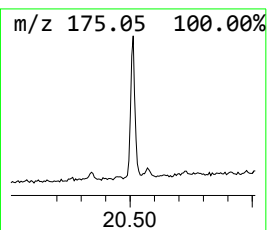
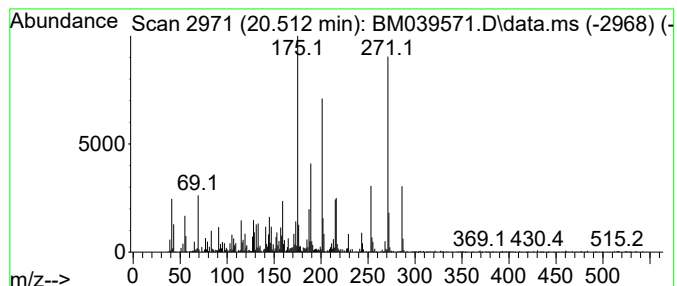
Instrument :
BNA_M
ClientSampleId :
EO-3-041923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.512	20.00 ng	642848	Chrysene-d12	21.430	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H300	000511-15-9	99
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H3202	015340-82-6	76
3	7H-[1,3,4]Thiadiazolo[3,2-a]pyri...	271	C9H9N3O3S2	1000350-95-4	53
4	Pisiferol	302	C20H3002	024035-36-7	27
5	phenol, 4-[2-(4-methoxyphenyl)et...	271	C15H13NO4	1000396-99-6	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042123\
Data File : BM039571.D
Acq On : 22 Apr 2023 03:06
Operator : CG/JU
Sample : 02426-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EO-3-041923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM041723.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
Longifolene	13.742	2.4	ng	220443	3	14.483	1816100	20.0
Benzophenone	15.848	3.5	ng	313630	3	14.483	1816100	20.0
n-Hexadecanoic ...	18.136	6.2	ng	633325	4	17.242	2047770	20.0
4H-Cyclopenta[d...]	18.313	3.3	ng	334367	4	17.242	2047770	20.0
2-Phenanthrenol...	20.512	20.0	ng	642848	5	21.430	642848	20.0