

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
 Data File : BF134407.D
 Acq On : 21 Jul 2023 18:27
 Operator : CG\JU
 Sample : 03638-11
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP2

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134407.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	4	10	20	rVB	175859	237806	21.78%	2.641%
2	5.087	506	510	516	rBV	17553	21976	2.01%	0.244%
3	5.475	573	576	586	rBV	977324	965240	88.38%	10.722%
4	6.475	742	746	759	rBV	1058022	967421	88.58%	10.746%
5	6.834	804	807	818	rBV	385089	354393	32.45%	3.936%
6	7.398	899	903	915	rBV	791583	624978	57.23%	6.942%
7	8.116	1021	1025	1028	rBV	559544	444750	40.72%	4.940%
8	9.192	1204	1208	1211	rBV	1388446	1092099	100.00%	12.131%
9	9.875	1320	1324	1327	rBV	584944	491117	44.97%	5.455%
10	10.016	1345	1348	1356	rBV	32267	41265	3.78%	0.458%
11	10.669	1455	1459	1472	rBV	777335	725329	66.42%	8.057%
12	11.369	1574	1578	1581	rBV	571736	496310	45.45%	5.513%
13	11.392	1581	1582	1587	rVB	46497	24983	2.29%	0.278%
14	11.898	1665	1668	1680	rVB3	62292	79765	7.30%	0.886%
15	11.986	1680	1683	1685	rBV2	12958	14408	1.32%	0.160%
16	12.592	1782	1786	1789	rBV	109105	105185	9.63%	1.168%
17	12.686	1799	1802	1808	rBV2	14737	19716	1.81%	0.219%
18	12.821	1819	1825	1829	rBV	104069	103084	9.44%	1.145%
19	12.963	1845	1849	1853	rBV	1102349	931334	85.28%	10.345%
20	13.039	1858	1862	1868	rVB4	7175	13205	1.21%	0.147%
21	13.151	1879	1881	1886	rVB	14762	13278	1.22%	0.147%
22	13.257	1895	1899	1907	rVB2	13637	18767	1.72%	0.208%
23	13.539	1943	1947	1949	rBV4	11099	13775	1.26%	0.153%
24	13.874	2001	2004	2007	rVB4	12392	15207	1.39%	0.169%
25	13.939	2007	2015	2023	rBV4	16757	55805	5.11%	0.620%
26	14.033	2026	2031	2034	rVV	393222	429015	39.28%	4.765%
27	14.057	2034	2035	2044	rVB	59037	39809	3.65%	0.442%
28	14.186	2053	2057	2059	rBV4	18407	20224	1.85%	0.225%
29	14.421	2092	2097	2100	rBV	15479	16670	1.53%	0.185%
30	15.092	2206	2211	2214	rBV	53838	83469	7.64%	0.927%
31	15.157	2219	2222	2227	rVB6	11216	16808	1.54%	0.187%
32	15.204	2227	2230	2233	rBV2	15025	15734	1.44%	0.175%
33	15.404	2261	2264	2270	rBV	32738	41948	3.84%	0.466%
34	15.474	2272	2276	2281	rVB	40816	58043	5.31%	0.645%
35	15.539	2281	2287	2292	rBV	286526	375566	34.39%	4.172%
36	17.086	2545	2550	2557	rBV3	16399	34334	3.14%	0.381%

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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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

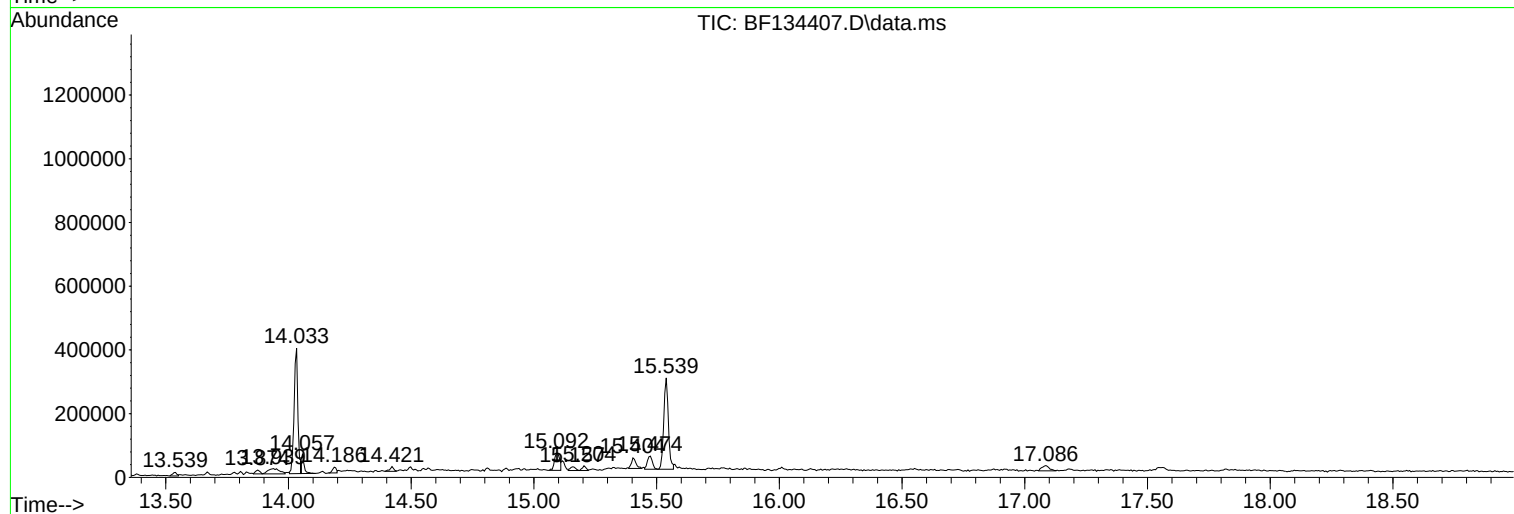
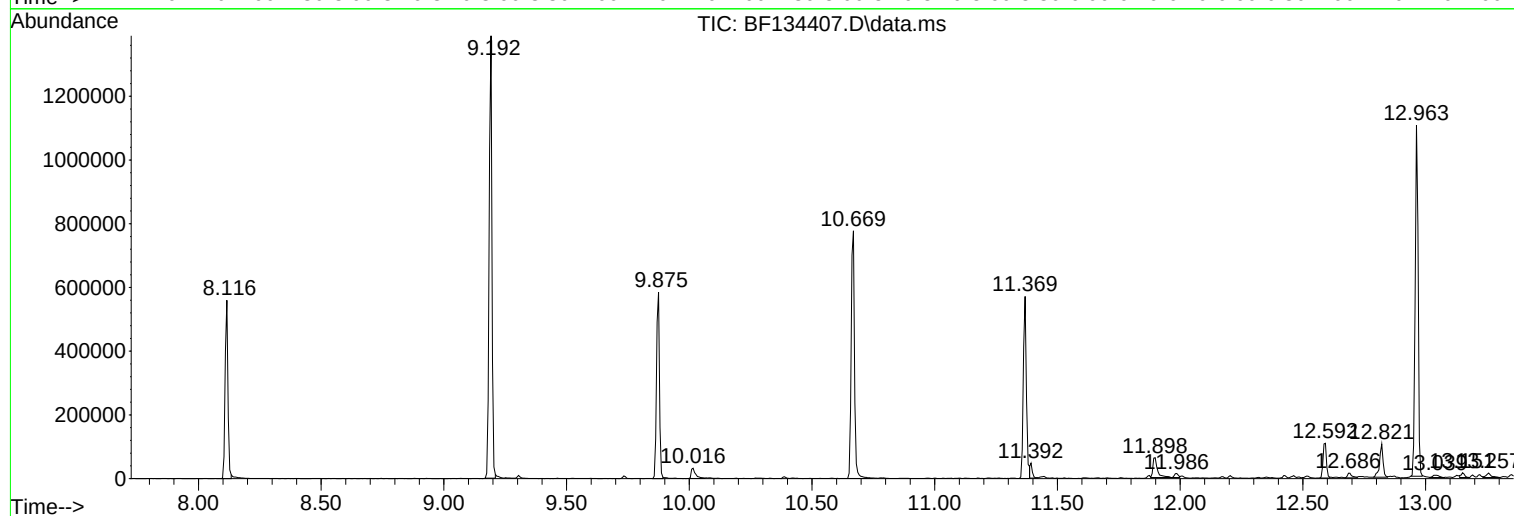
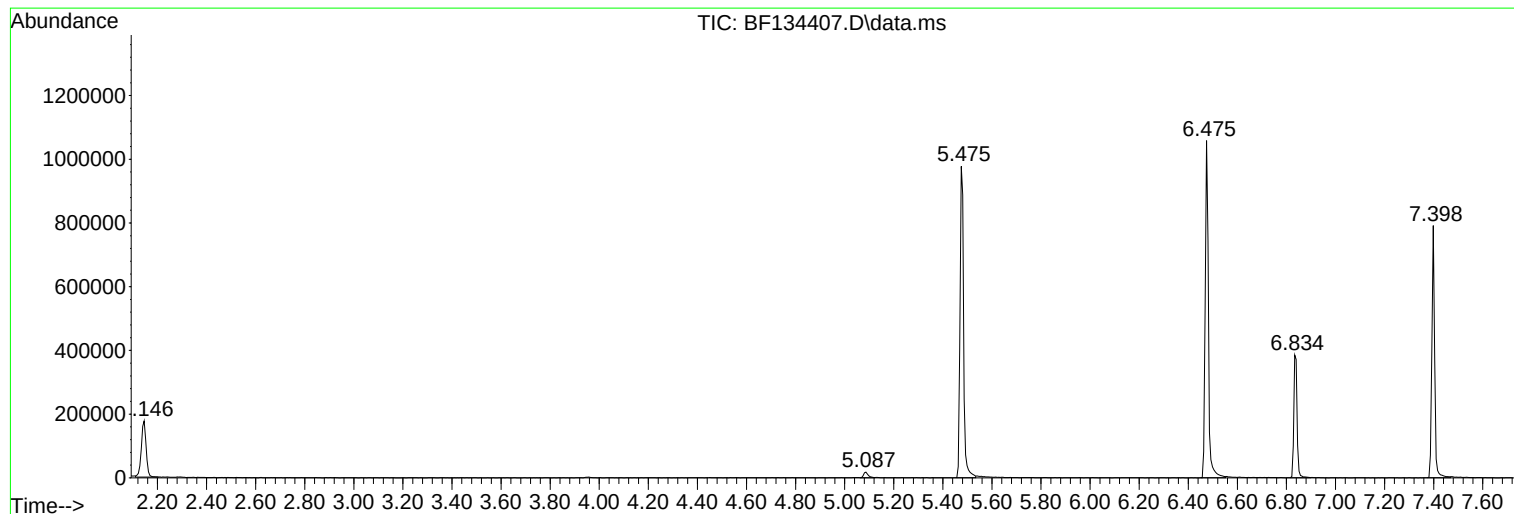
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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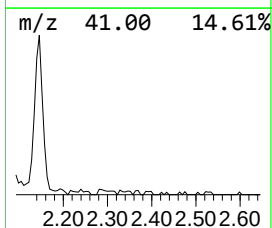
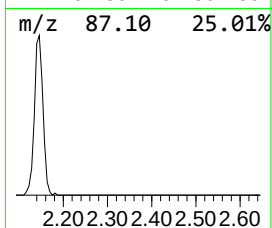
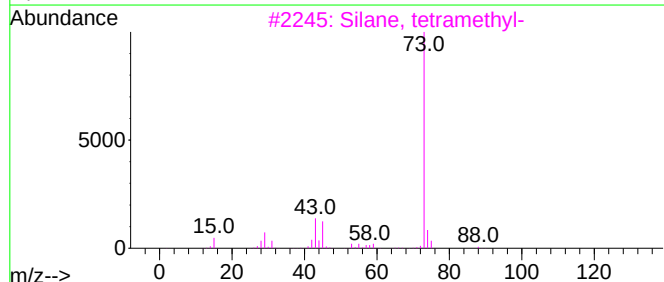
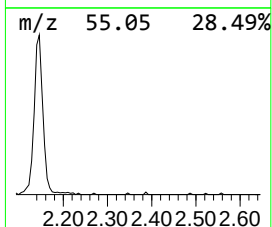
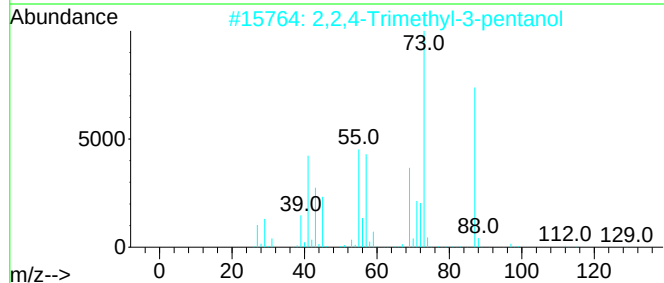
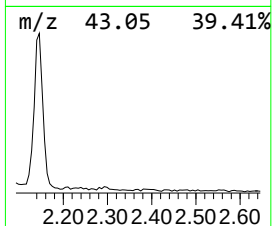
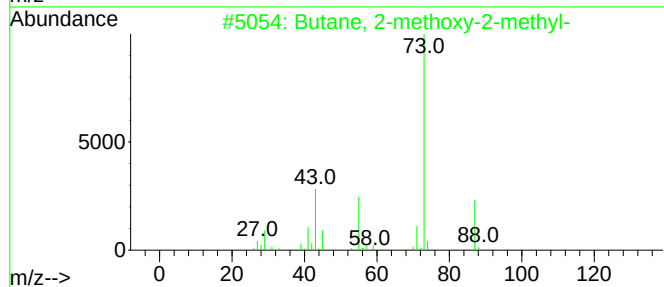
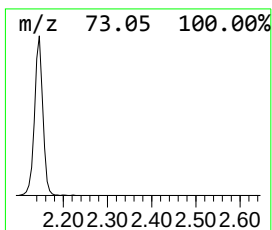
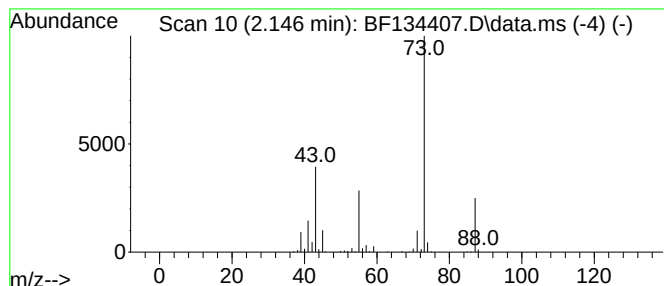
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
2.146	13.42 ng	237806	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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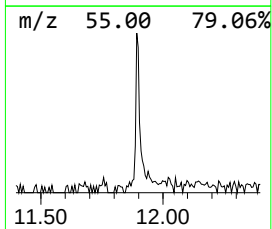
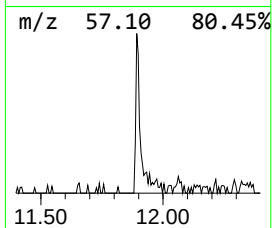
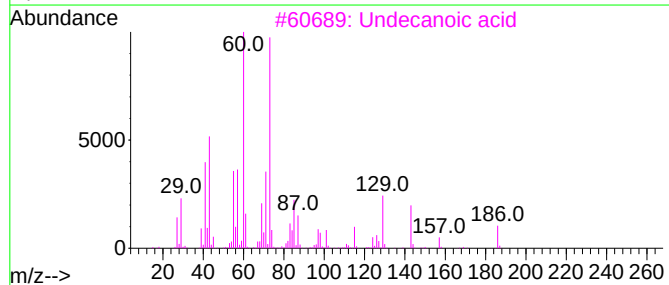
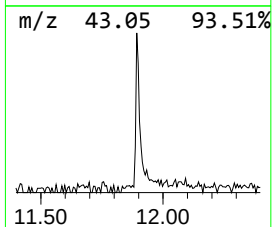
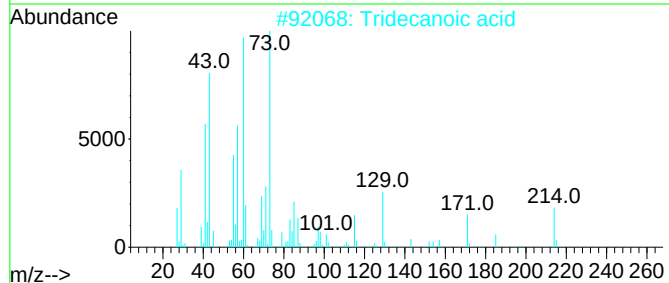
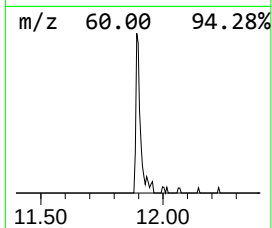
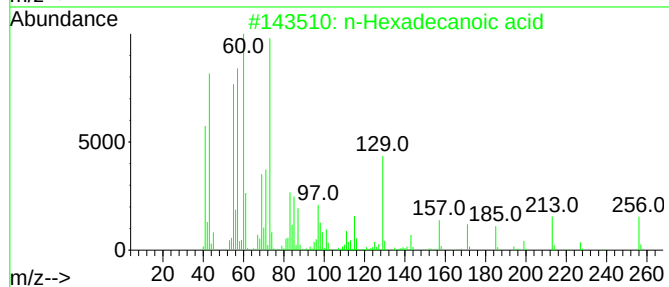
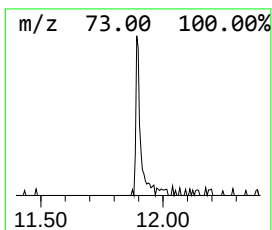
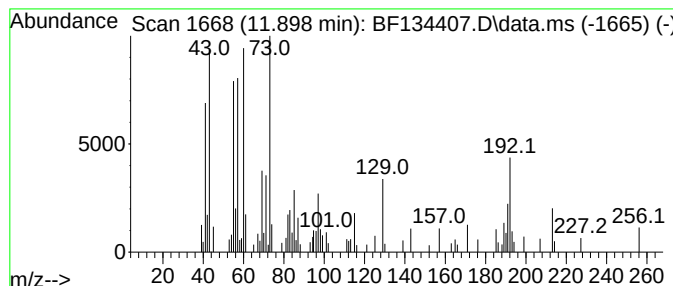
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	3.21 ng	79765	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Undecanoic acid	186	C11H22O2	000112-37-8	55
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	49



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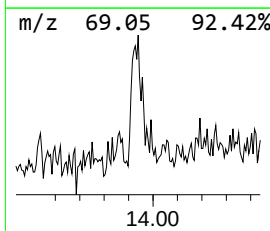
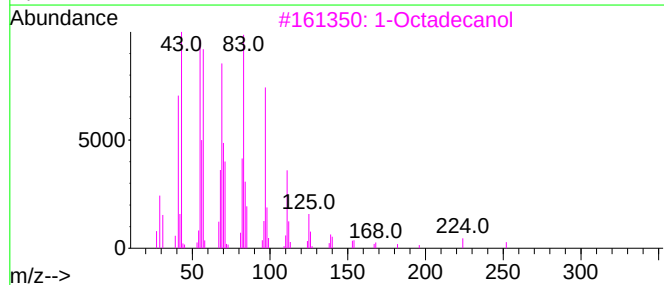
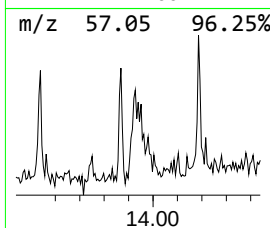
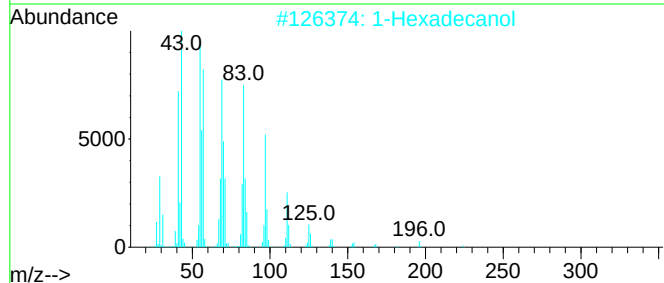
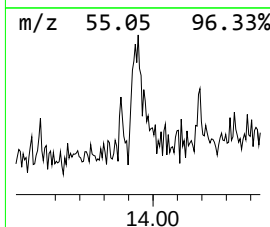
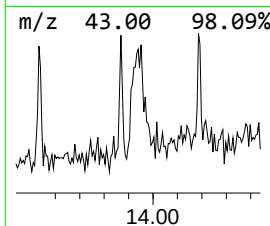
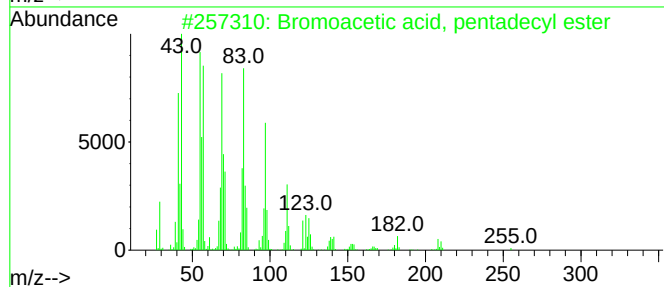
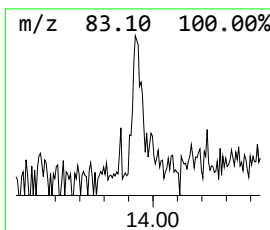
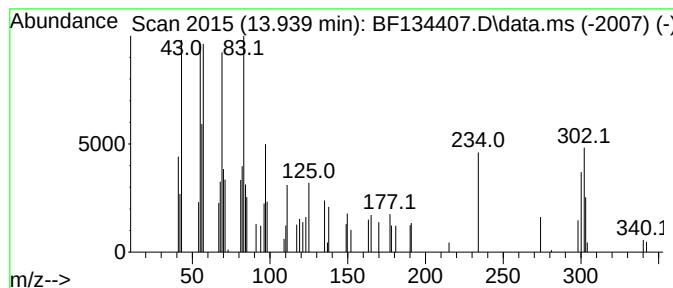
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Bromoacetic acid, pentadecy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	2.60 ng	55805	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	89
2			1-Hexadecanol	242	C16H34O	036653-82-4	55
3			1-Octadecanol	270	C18H38O	000112-92-5	49
4			9-Octadecene, (E)-	252	C18H36	007206-25-9	49
5			Cyclohexadecane	224	C16H32	000295-65-8	49



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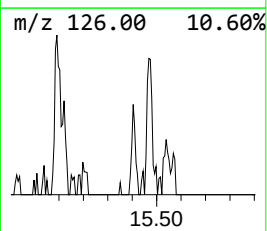
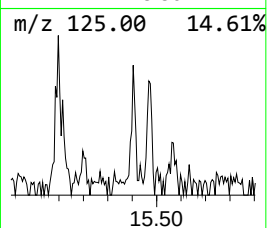
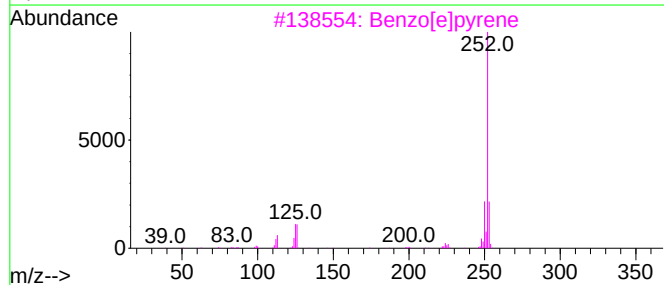
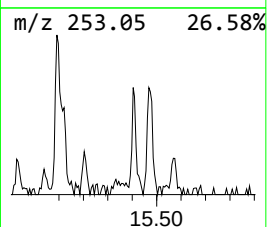
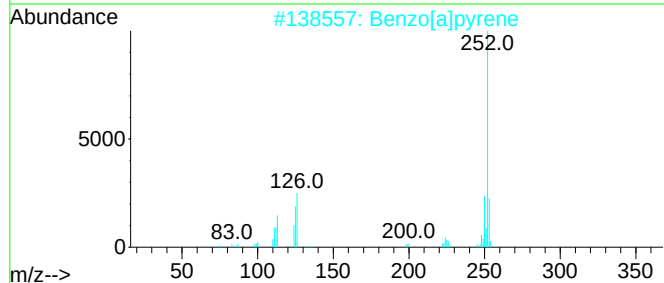
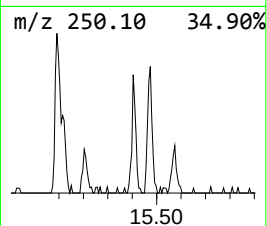
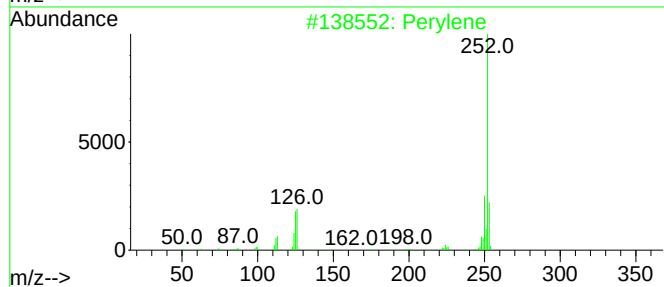
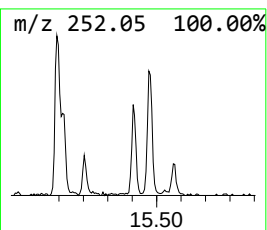
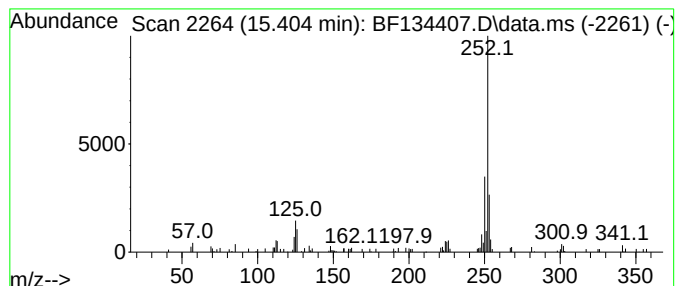
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	2.23 ng	41948	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	93
2			Benzo[a]pyrene	252	C20H12	000050-32-8	89
3			Benzo[e]pyrene	252	C20H12	000192-97-2	89
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	76
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	76



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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...	2.146	13.4	ng	237806	1	6.840	354393	20.0
n-Hexadecanoic ...	11.898	3.2	ng	79765	4	11.369	496310	20.0
Bromoacetic aci...	13.939	2.6	ng	55805	5	14.033	429015	20.0
Perylene	15.404	2.2	ng	41948	6	15.539	375566	20.0