

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110323\
 Data File : BF136128.D
 Acq On : 03 Nov 2023 17:09
 Operator : CG\JU
 Sample : 05141-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-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-BF103023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136128.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.045	498	503	509	rBV	68570	78181	4.26%	0.533%
2	5.445	566	571	574	rBV	1736562	1565664	85.28%	10.672%
3	6.445	736	741	744	rBV	1565357	1577243	85.91%	10.751%
4	6.816	801	804	808	rVB	824918	633979	34.53%	4.321%
5	7.375	895	899	903	rBV	1118025	1052157	57.31%	7.172%
6	8.098	1018	1022	1025	rBV	1066155	816414	44.47%	5.565%
7	9.175	1202	1205	1209	rBV	2165754	1835874	100.00%	12.514%
8	9.857	1317	1321	1324	rBV	1121460	860500	46.87%	5.865%
9	10.645	1451	1455	1458	rBV	1258238	992732	54.07%	6.767%
10	11.345	1570	1574	1577	rBV	868952	776018	42.27%	5.290%
11	11.369	1577	1578	1582	rVB	92334	54458	2.97%	0.371%
12	11.886	1662	1666	1670	rBV2	114985	108189	5.89%	0.737%
13	12.563	1778	1781	1785	rBV	149007	128873	7.02%	0.878%
14	12.663	1795	1798	1799	rBV2	38680	33947	1.85%	0.231%
15	12.768	1812	1816	1817	rBV2	43587	42912	2.34%	0.293%
16	12.792	1817	1820	1824	rVB	136650	134807	7.34%	0.919%
17	12.945	1842	1846	1850	rVB	1802982	1484091	80.84%	10.116%
18	13.192	1882	1888	1891	rBV2	24191	25912	1.41%	0.177%
19	13.868	2000	2003	2016	rBV5	41978	122599	6.68%	0.836%
20	14.004	2020	2026	2029	rVV	763226	791892	43.13%	5.398%
21	14.027	2029	2030	2036	rVB	86023	58125	3.17%	0.396%
22	14.186	2054	2057	2060	rBV2	29038	24477	1.33%	0.167%
23	14.492	2105	2109	2112	rBV2	33391	39319	2.14%	0.268%
24	14.809	2160	2163	2168	rVB2	24750	29551	1.61%	0.201%
25	15.051	2199	2204	2207	rBV	85625	126587	6.90%	0.863%
26	15.162	2219	2223	2227	rVB	38880	45864	2.50%	0.313%
27	15.362	2252	2257	2263	rVB	49525	64127	3.49%	0.437%
28	15.421	2263	2267	2273	rVB	69308	90585	4.93%	0.617%
29	15.492	2273	2279	2287	rBV	673519	834818	45.47%	5.690%
30	15.556	2287	2290	2297	rVB3	18486	31347	1.71%	0.214%
31	16.015	2365	2368	2374	rVB2	15534	23174	1.26%	0.158%
32	16.551	2455	2459	2464	rBV6	12186	23304	1.27%	0.159%
33	16.992	2528	2534	2543	rVB3	32313	72515	3.95%	0.494%
34	17.186	2560	2567	2573	rBV6	16485	37528	2.04%	0.256%
35	17.445	2606	2611	2620	rVB2	26569	52852	2.88%	0.360%

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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-BF103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

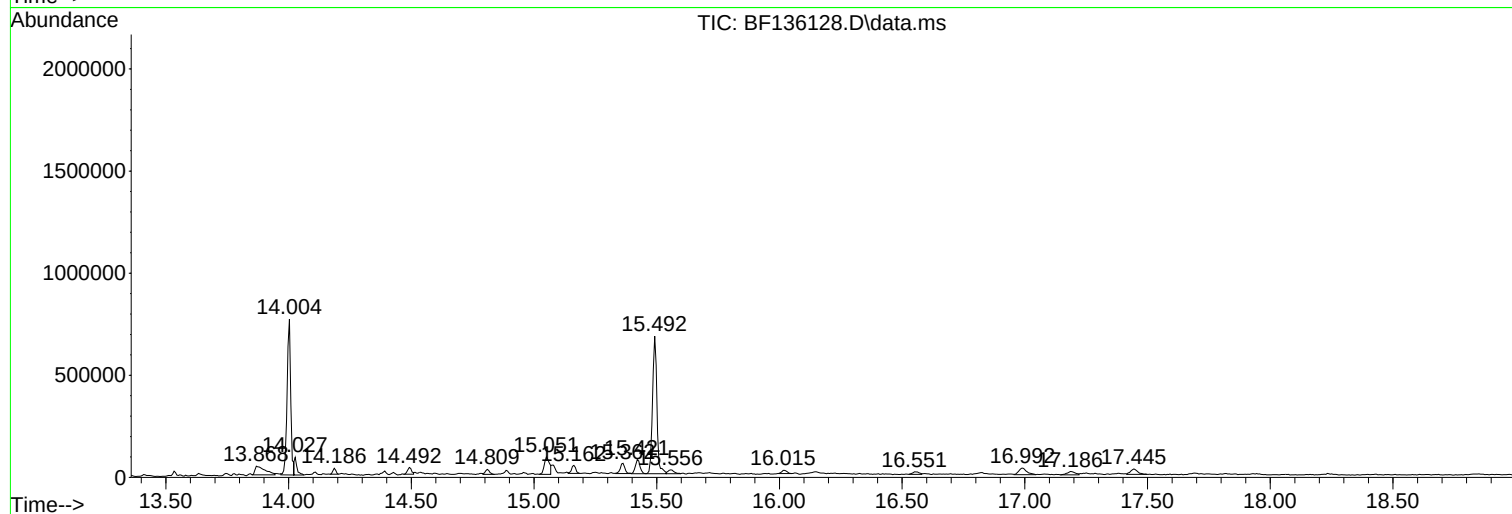
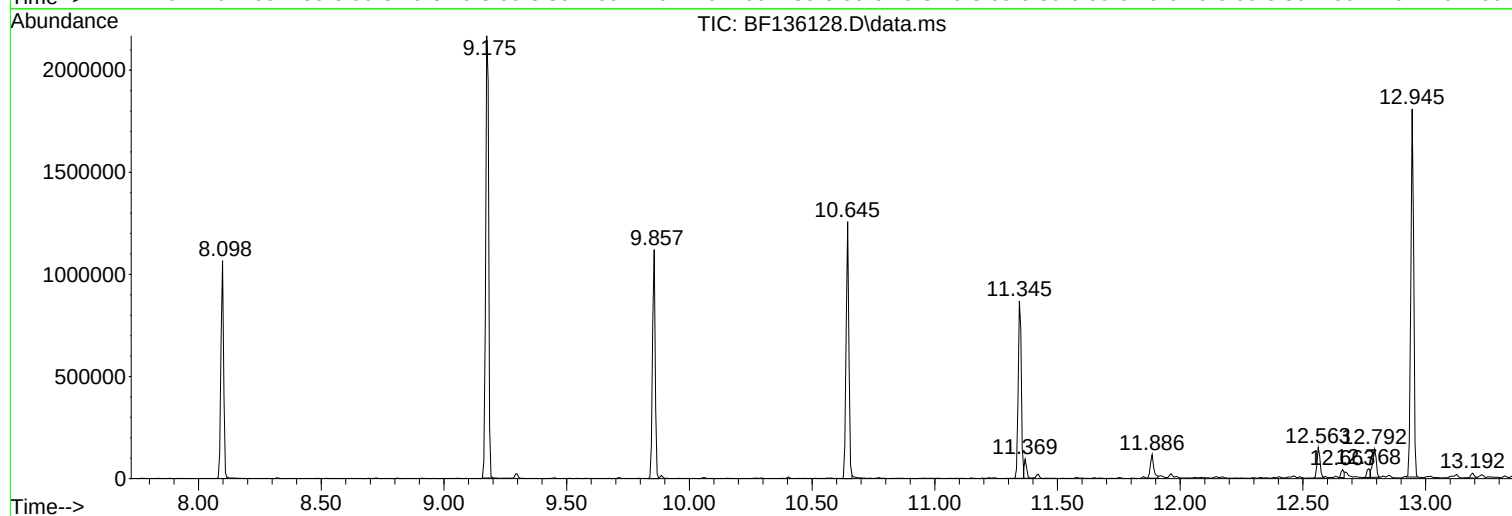
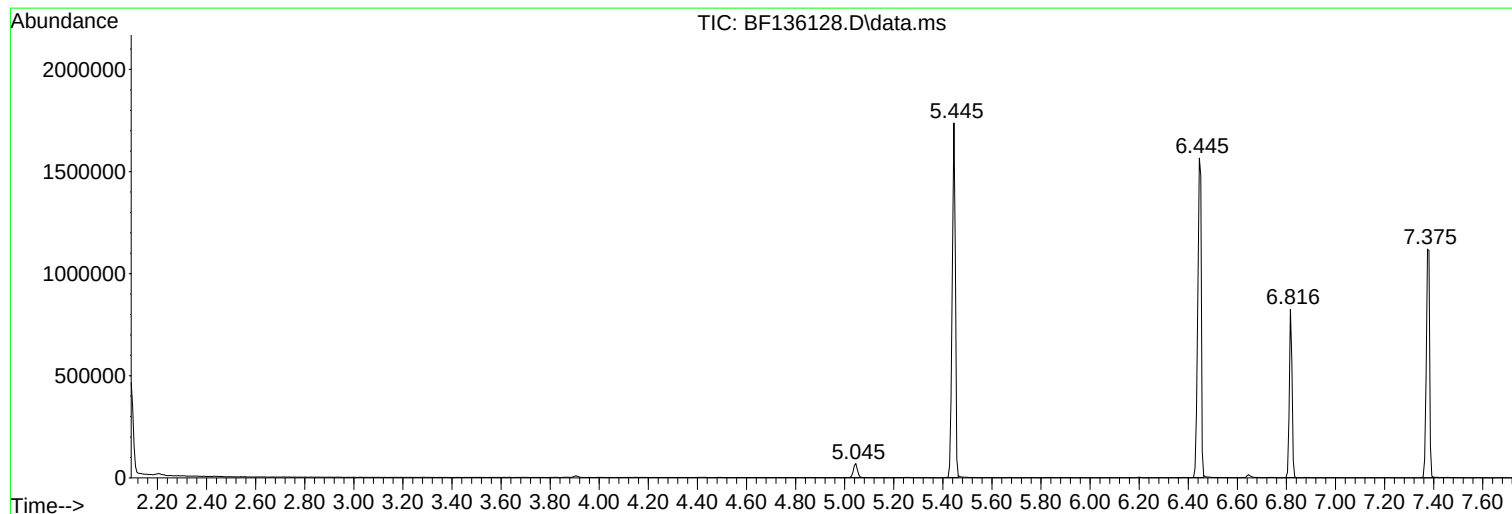
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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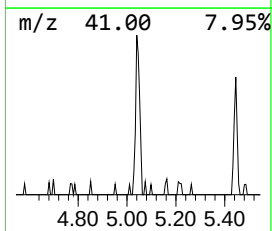
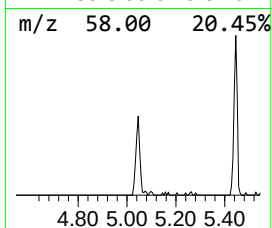
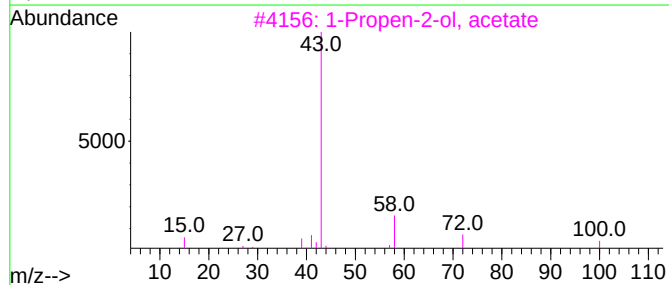
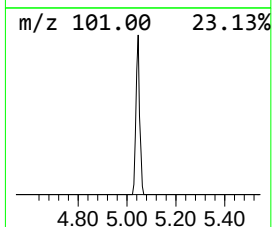
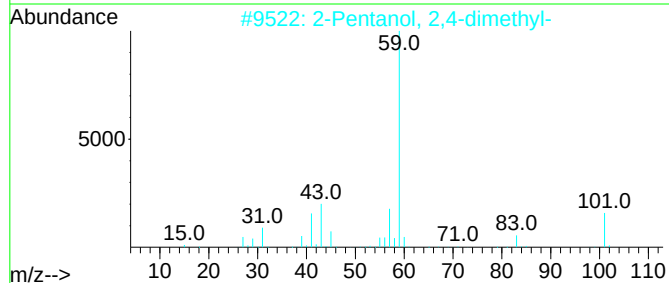
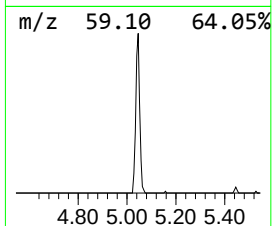
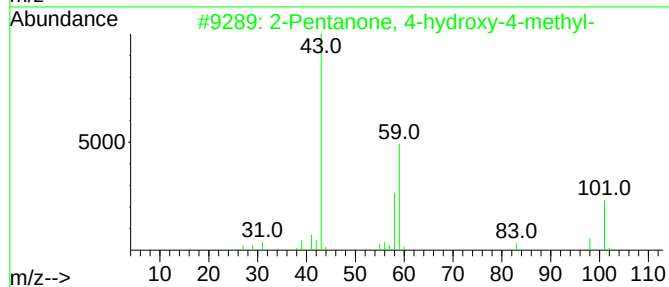
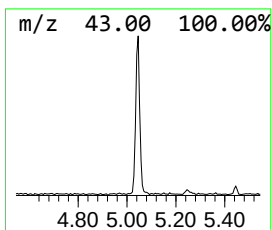
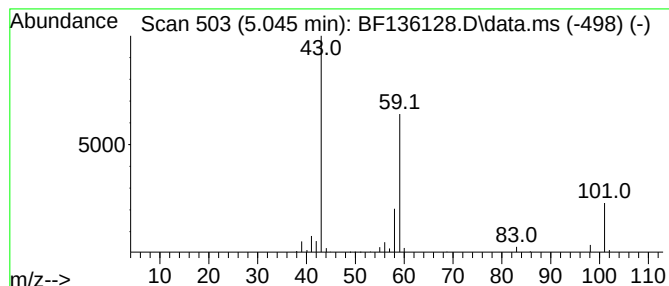
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	2.47 ng	78181	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	17		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	2,3-Butanediol, 2,3-dimethyl-	118	C6H14O2	000076-09-5	12		
5	Acetone	58	C3H6O	000067-64-1	9		



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ClientSampleId :
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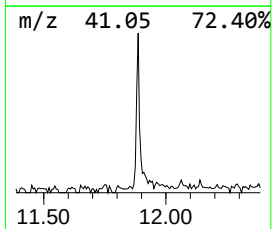
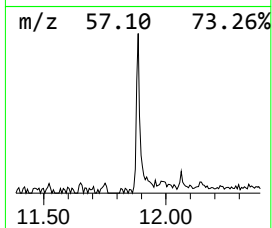
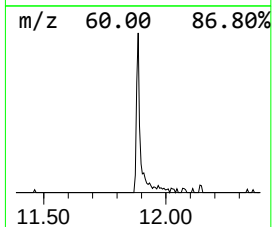
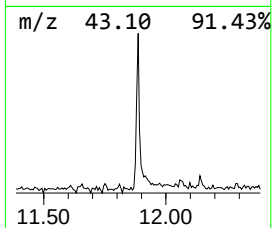
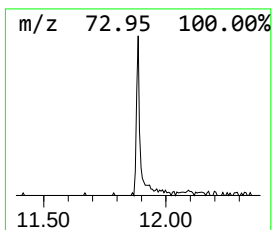
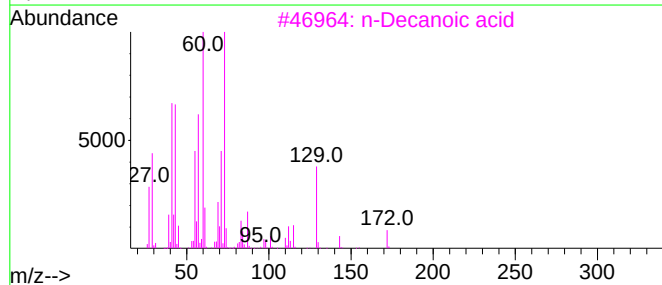
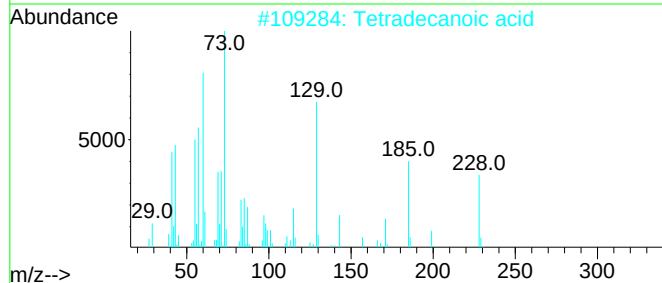
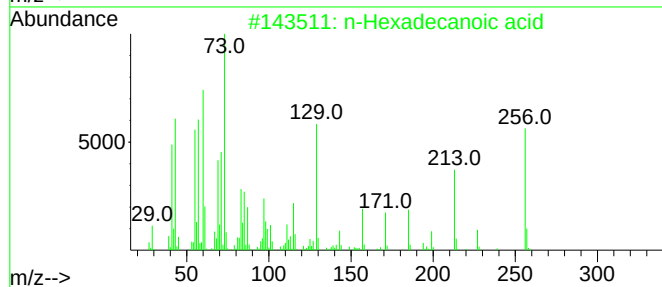
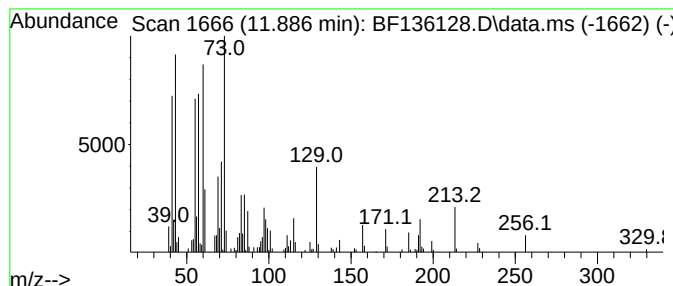
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	2.79 ng	108189	Phenanthrene-d10	11.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
3			n-Decanoic acid	172	C10H20O2	000334-48-5	76
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	74



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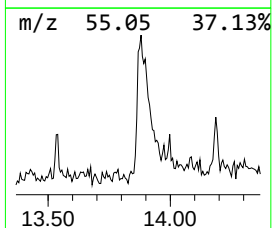
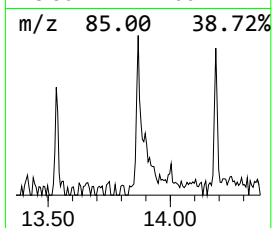
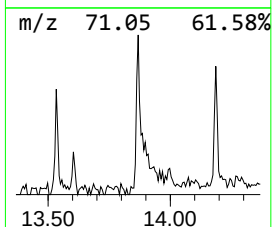
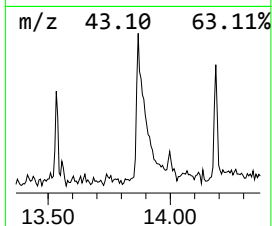
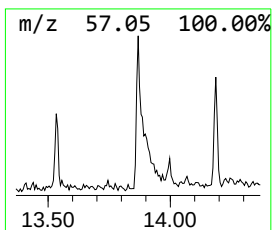
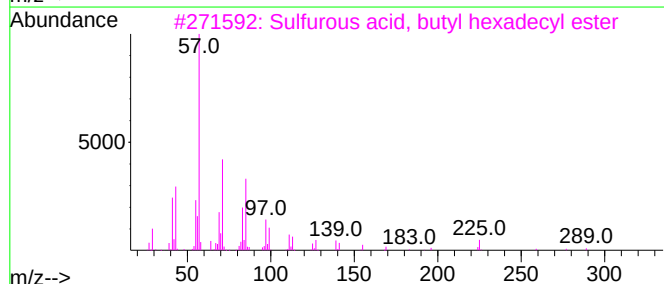
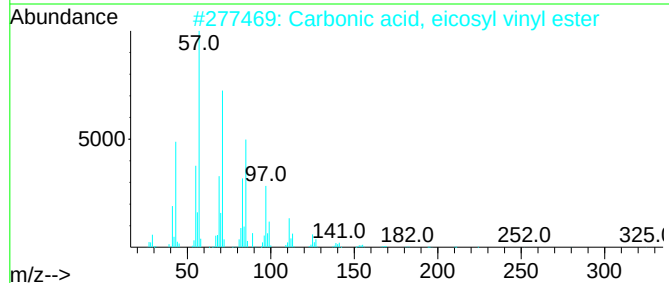
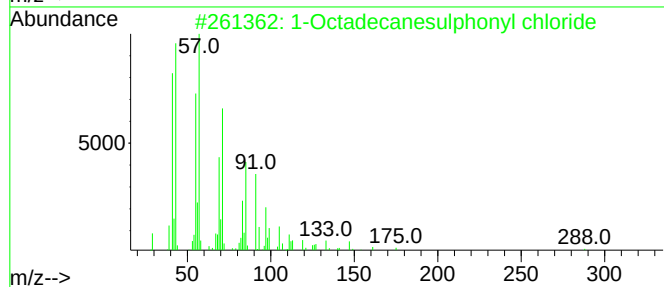
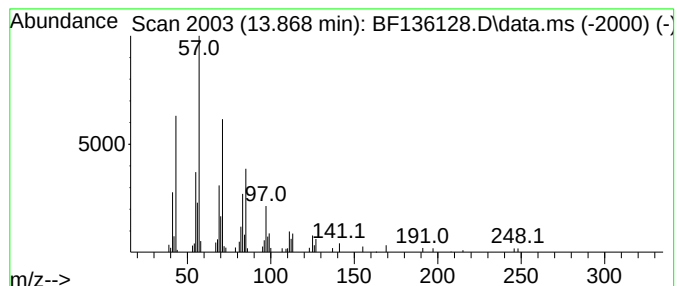
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Octadecanesulphonyl chloride Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.868	3.10 ng	122599	Chrysene-d12	14.004		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
2		Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	90
3		Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	90
4		Tetracontane, 3,5,24-trimethyl-	605	C43H88	055162-61-3	90
5		Carbonic acid, tridecyl vinyl ester	270	C16H30O3	1000382-54-7	90



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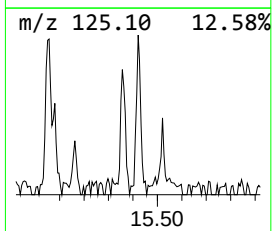
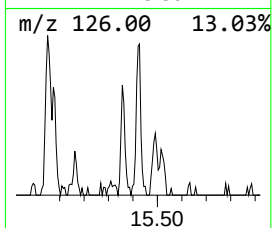
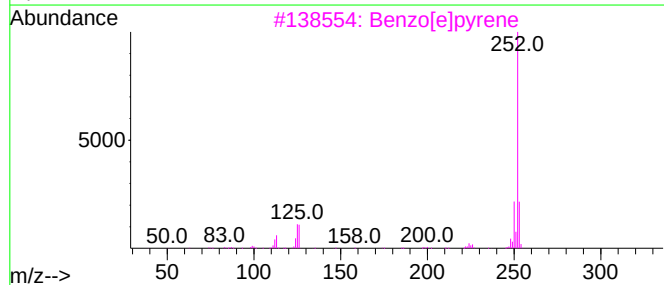
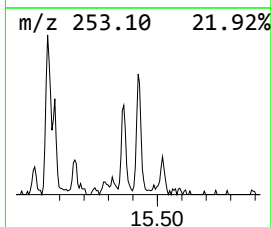
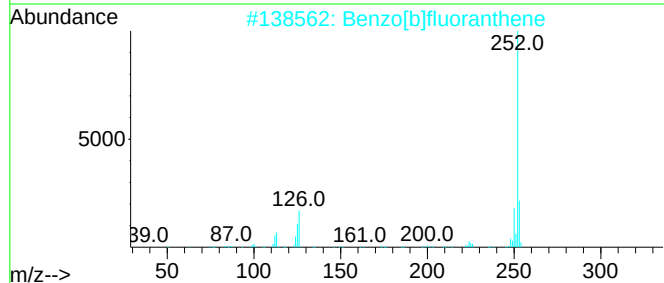
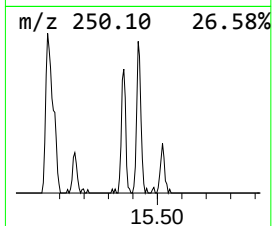
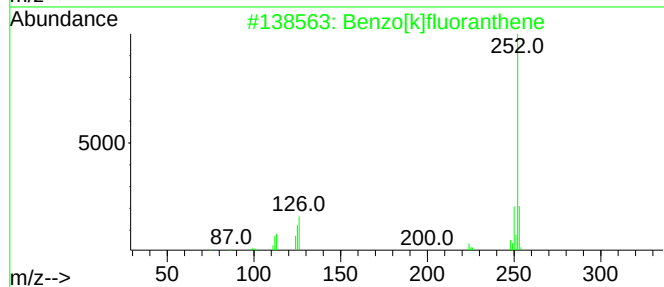
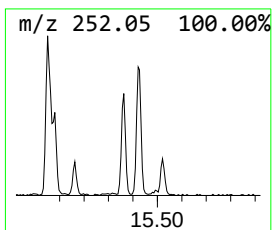
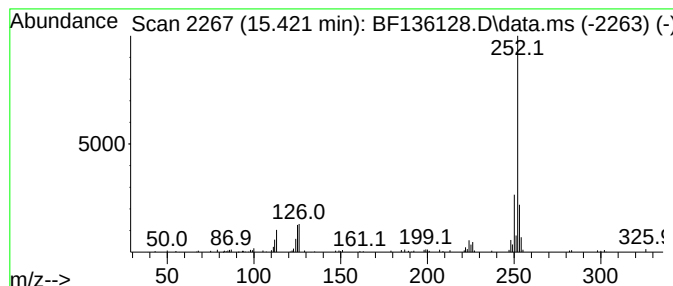
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.421	2.17 ng	90585	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
3			Benzo[e]pyrene	252	C20H12	000192-97-2	94
4			Benzo[a]pyrene	252	C20H12	000050-32-8	93
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	89



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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
2-Pentanone, 4-...	5.045	2.5	ng	78181	1	6.816	633979	20.0
n-Hexadecanoic ...	11.886	2.8	ng	108189	4	11.345	776018	20.0
1-Octadecanesul...	13.868	3.1	ng	122599	5	14.004	791892	20.0
Benzo[e]pyrene	15.421	2.2	ng	90585	6	15.492	834818	20.0