

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121823\
 Data File : BF136617.D
 Acq On : 18 Dec 2023 16:34
 Operator : CG\JU
 Sample : 05833-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 351

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-BF120523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136617.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	495	498	507	rVB	118859	144971	6.26%	0.979%
2	5.428	564	568	571	rBV	1977035	1743381	75.24%	11.767%
3	6.434	734	739	742	rBV	1922528	1708655	73.74%	11.533%
4	6.787	795	799	802	rBV	777019	579391	25.00%	3.911%
5	7.345	889	894	897	rBV	1219527	1138230	49.12%	7.683%
6	8.063	1012	1016	1019	rBV	959247	749999	32.37%	5.062%
7	9.145	1195	1200	1203	rBV	2605216	2317142	100.00%	15.640%
8	9.822	1311	1315	1318	rBV	994284	781273	33.72%	5.273%
9	10.616	1445	1450	1460	rBV	1215952	1133014	48.90%	7.648%
10	11.310	1565	1568	1571	rBV	788997	677195	29.23%	4.571%
11	11.333	1571	1572	1576	rVB	44040	28715	1.24%	0.194%
12	11.845	1656	1659	1669	rBV	170116	184747	7.97%	1.247%
13	12.527	1772	1775	1779	rBV	97907	89972	3.88%	0.607%
14	12.639	1790	1794	1799	rBV4	37411	52959	2.29%	0.357%
15	12.757	1808	1814	1817	rBV	90781	96554	4.17%	0.652%
16	12.910	1836	1840	1843	rBV	1994611	1695982	73.19%	11.448%
17	13.869	1998	2003	2012	rBV7	44695	134689	5.81%	0.909%
18	13.969	2014	2020	2023	rVV	581757	683081	29.48%	4.611%
19	13.992	2023	2024	2031	rVB	65647	45682	1.97%	0.308%
20	14.827	2164	2166	2169	rVB3	29108	25752	1.11%	0.174%
21	15.010	2194	2197	2201	rBV	64688	97056	4.19%	0.655%
22	15.316	2247	2249	2255	rVB	42131	55071	2.38%	0.372%
23	15.451	2267	2272	2276	rBV	534617	651742	28.13%	4.399%

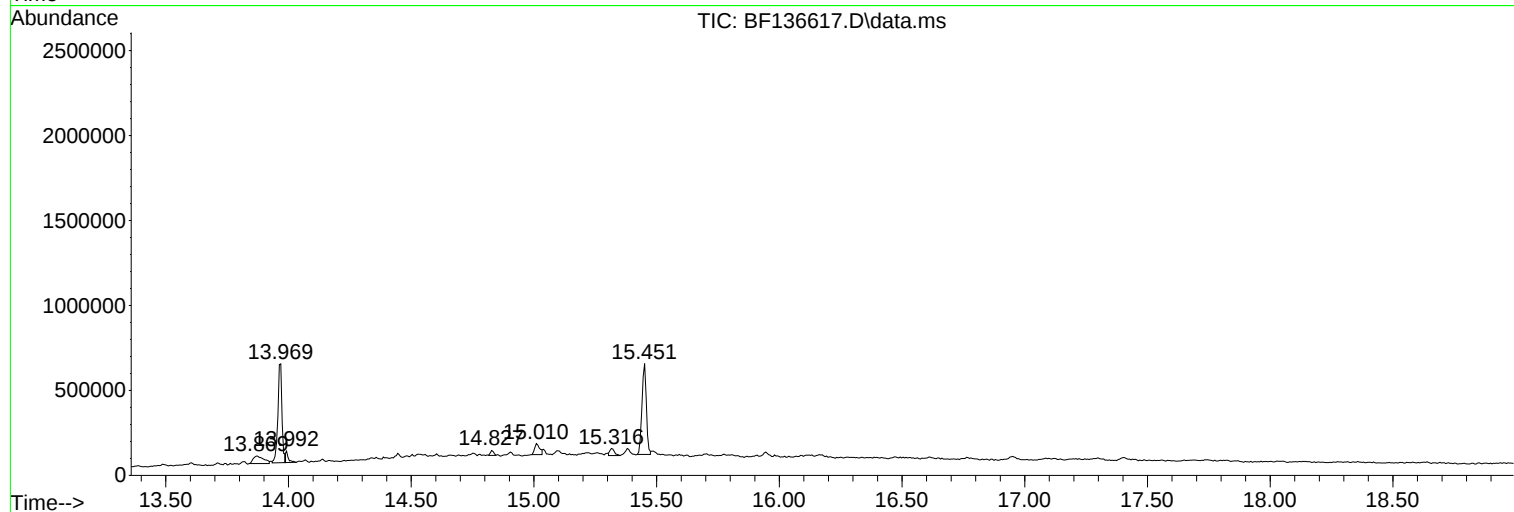
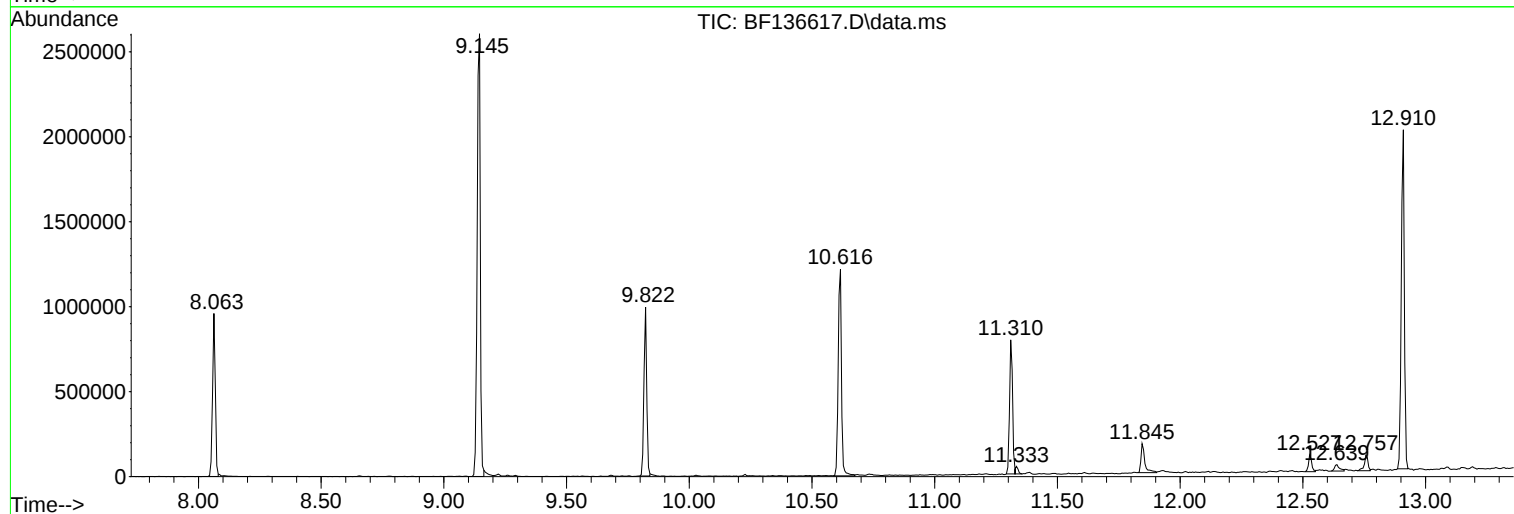
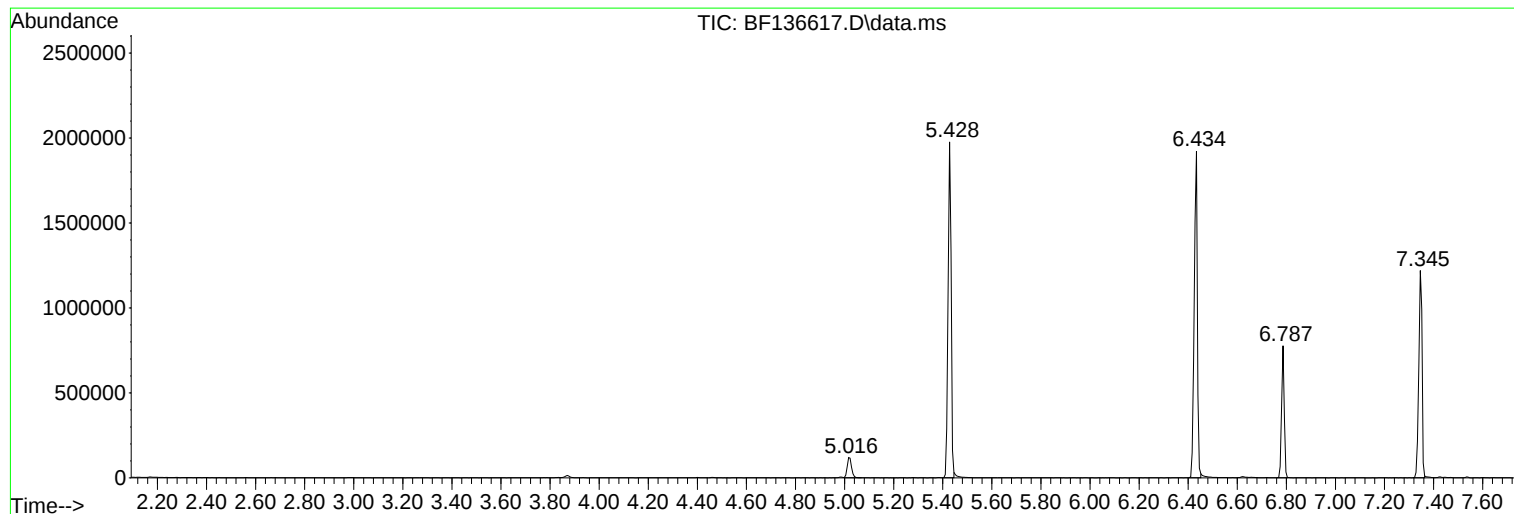
Sum of corrected areas: 14815253

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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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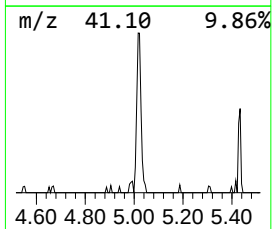
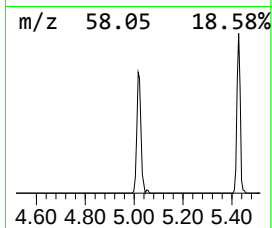
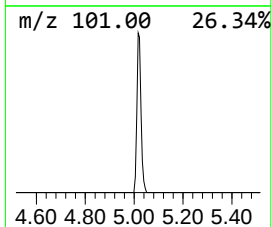
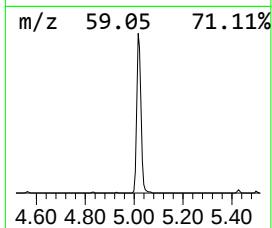
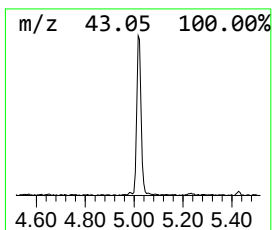
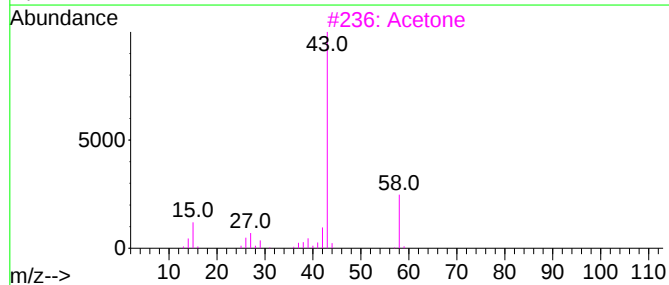
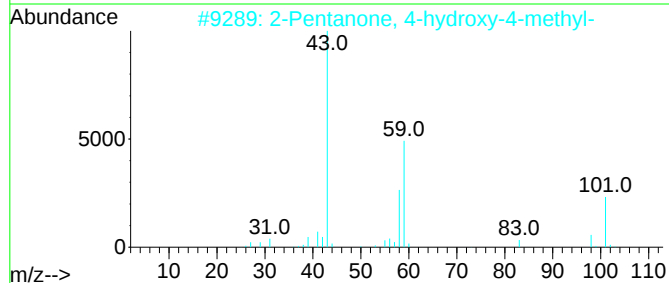
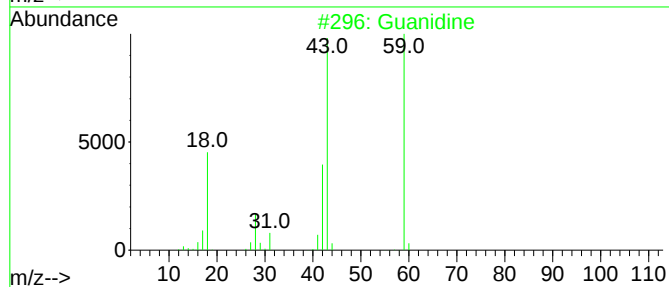
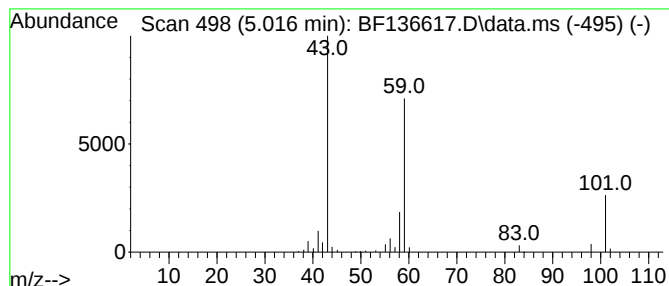
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown5.016 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	5.00 ng	144971	1,4-Dichlorobenzene-d4	6.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Guanidine	59	CH5N3	000113-00-8	43
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3			Acetone	58	C3H6O	000067-64-1	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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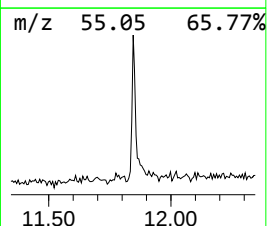
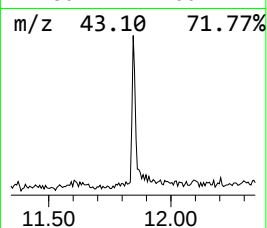
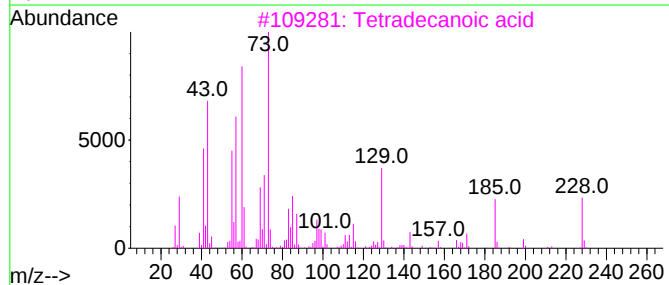
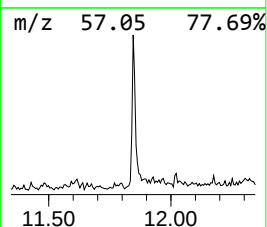
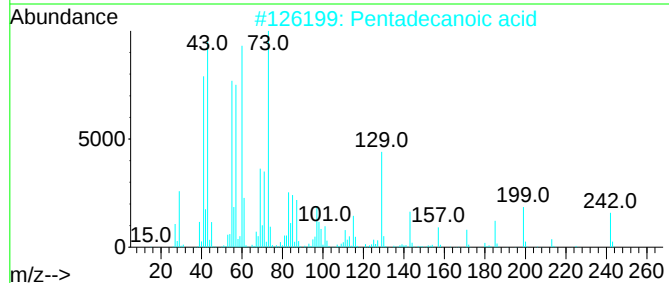
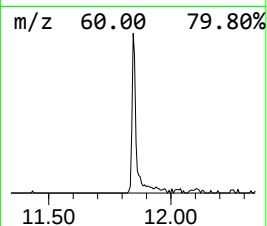
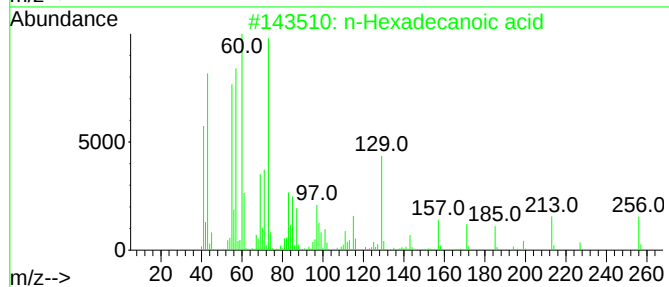
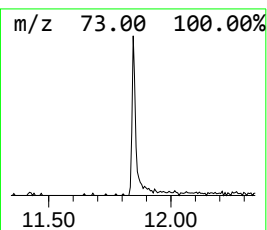
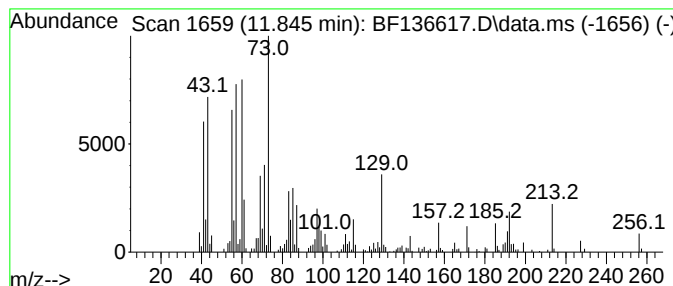
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	5.46 ng	184747	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	46



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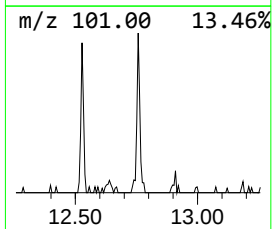
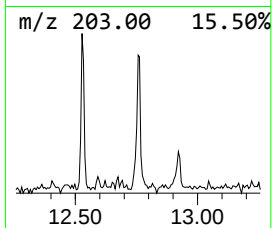
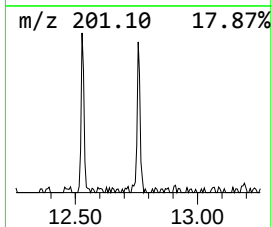
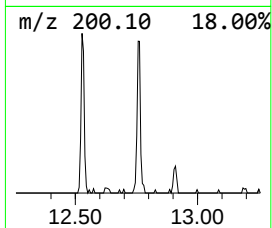
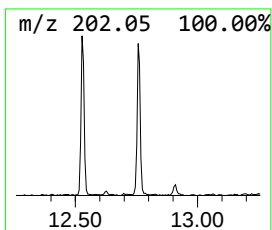
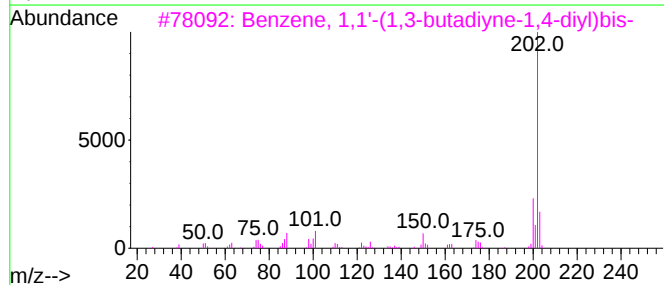
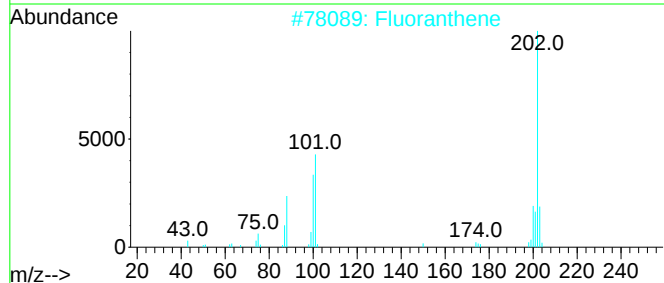
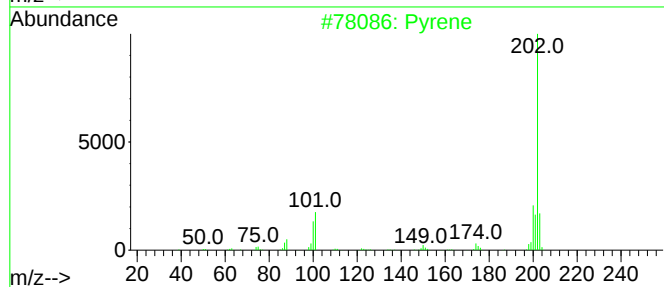
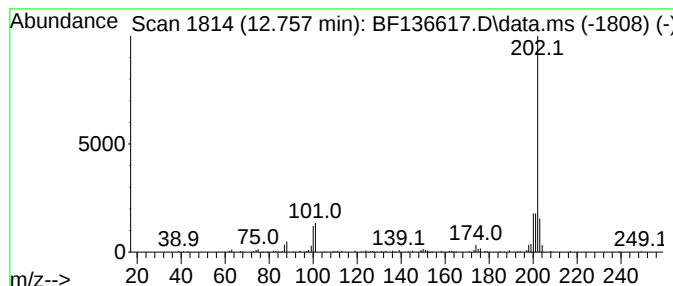
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Peak Number 3 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.757	2.83 ng	96554	Chrysene-d12	13.969	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene	202	C16H10	000129-00-0	93
2	Fluoranthene	202	C16H10	000206-44-0	93
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	72
4	1,4-naphthalenedione, 2-ethoxy-	202	C12H10O3	1000400-43-2	40
5	4-Methoxy-naphthalene-1-carboxyl...	202	C12H10O3	1000317-85-4	40



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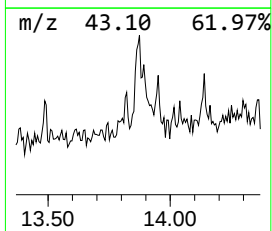
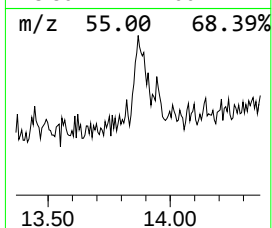
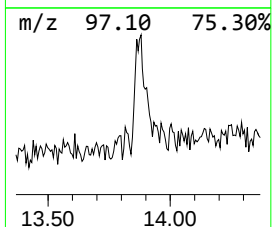
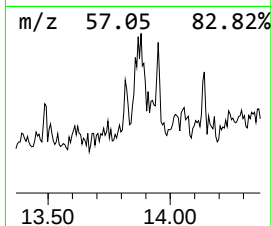
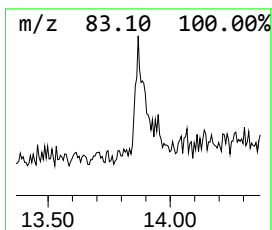
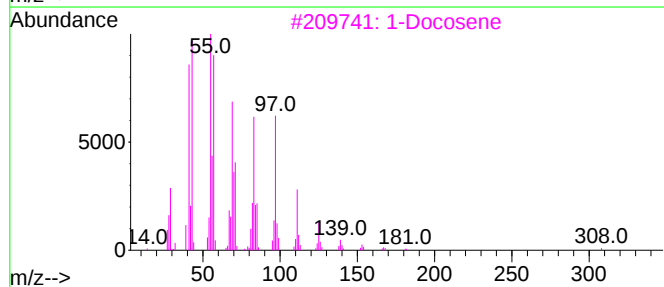
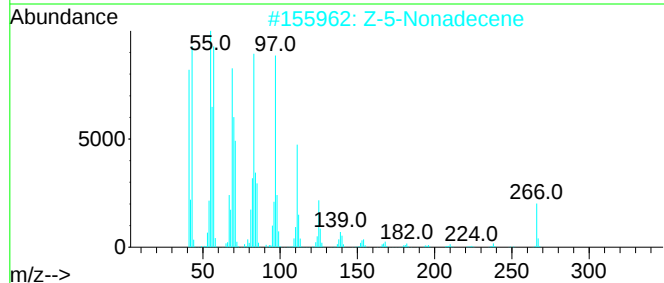
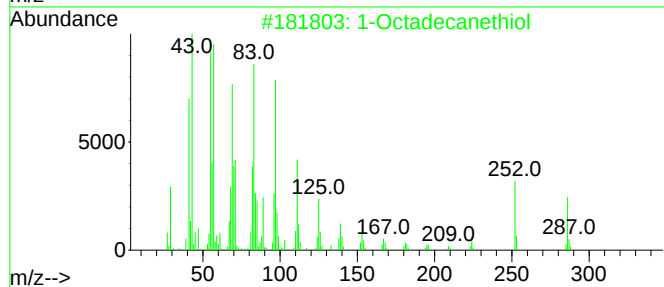
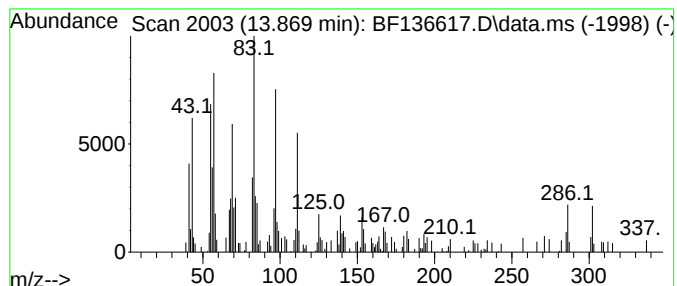
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Peak Number 4 1-Octadecanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.868	3.94 ng	134689	Chrysene-d12	13.969	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanethiol	286	C18H38S	002885-00-9	72
2	Z-5-Nonadecene	266	C19H38	1000131-11-8	62
3	1-Docosene	308	C22H44	001599-67-3	62
4	Triacontan-15-ol	438	C30H62O	031849-26-0	53
5	1-Pentadecene	210	C15H30	013360-61-7	49



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown5.016	5.016	5.0	ng	144971	1	6.787	579391	20.0
n-Hexadecanoic ...	11.845	5.5	ng	184747	4	11.310	677195	20.0
Benzene, 1,1'-(...	12.757	2.8	ng	96554	5	13.969	683081	20.0
1-Octadecanethiol	13.868	3.9	ng	134689	5	13.969	683081	20.0