

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031921\
 Data File : BG048434.D
 Acq On : 19 Mar 2021 21:48
 Operator : CG/JU
 Sample : M1721-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TR-05-031821

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_G\METHODS\8270-BG031821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048434.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.768	66	73	81	rBV	63885	101289	3.41%	0.588%
2	5.183	308	314	321	rVB2	17782	30678	1.03%	0.178%
3	5.654	387	394	403	rBV	796946	1268656	42.70%	7.365%
4	7.252	659	666	677	rVB	825616	1479687	49.80%	8.590%
5	8.109	804	812	818	rBV	214268	346500	11.66%	2.012%
6	9.273	1000	1010	1019	rBV	523335	927563	31.22%	5.385%
7	10.930	1284	1292	1299	rBV	256724	465320	15.66%	2.701%
8	13.374	1700	1708	1714	rBV	1198002	1897496	63.87%	11.016%
9	14.191	1842	1847	1853	rBV	70724	101325	3.41%	0.588%
10	14.379	1875	1879	1887	rVB6	14153	30695	1.03%	0.178%
11	14.749	1935	1942	1948	rVB	429603	665225	22.39%	3.862%
12	16.235	2188	2195	2206	rBV	1259387	1919594	64.61%	11.144%
13	17.498	2404	2410	2415	rBV	579228	877548	29.54%	5.095%
14	17.540	2415	2417	2426	rVV	74253	107273	3.61%	0.623%
15	17.628	2428	2432	2441	rVB5	15774	38037	1.28%	0.221%
16	18.380	2554	2560	2564	rBV2	210600	289512	9.74%	1.681%
17	18.568	2587	2592	2597	rBV6	21435	45090	1.52%	0.262%
18	18.909	2645	2650	2655	rVB6	29770	54609	1.84%	0.317%
19	19.149	2687	2691	2696	rBV	105519	128600	4.33%	0.747%
20	19.549	2754	2759	2765	rVB	173177	269208	9.06%	1.563%
21	19.649	2772	2776	2782	rBV9	51857	83537	2.81%	0.485%
22	19.784	2796	2799	2803	rBV5	29318	44180	1.49%	0.256%
23	19.913	2817	2821	2829	rVB	154270	231902	7.81%	1.346%
24	20.107	2848	2854	2861	rBV	2346421	2971046	100.00%	17.249%
25	20.254	2872	2879	2882	rVB8	46597	73023	2.46%	0.424%
26	21.417	3073	3077	3088	rVV6	163420	297570	10.02%	1.728%
27	21.506	3089	3092	3098	rVB5	55754	80782	2.72%	0.469%
28	21.793	3133	3141	3146	rBV	619557	1141575	38.42%	6.627%
29	21.840	3146	3149	3158	rVB2	70466	121211	4.08%	0.704%
30	24.819	3650	3656	3663	rVB4	29625	83550	2.81%	0.485%
31	24.960	3678	3680	3688	rVB	42228	79057	2.66%	0.459%
32	25.131	3699	3709	3718	rBV3	338690	973573	32.77%	5.652%

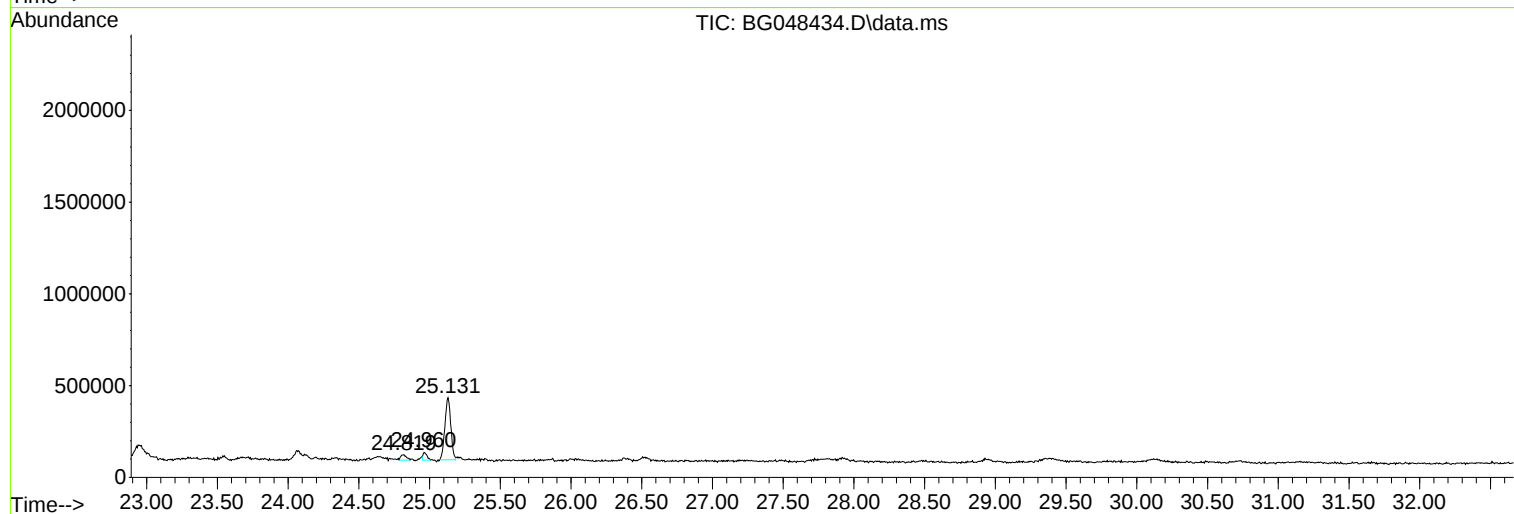
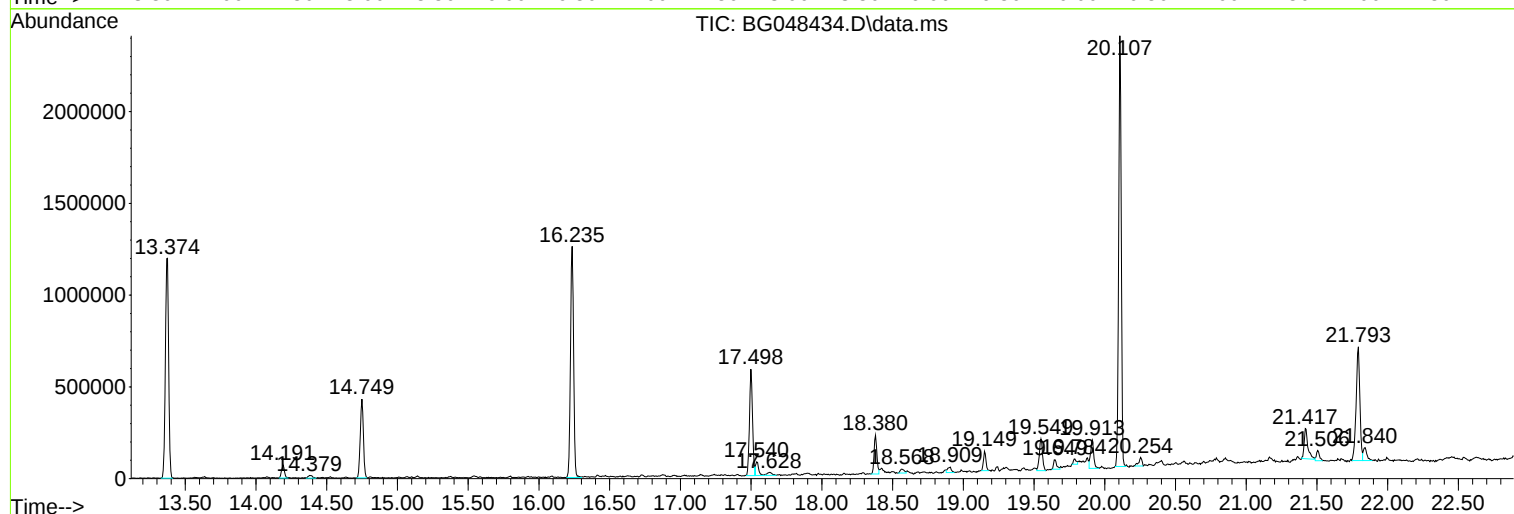
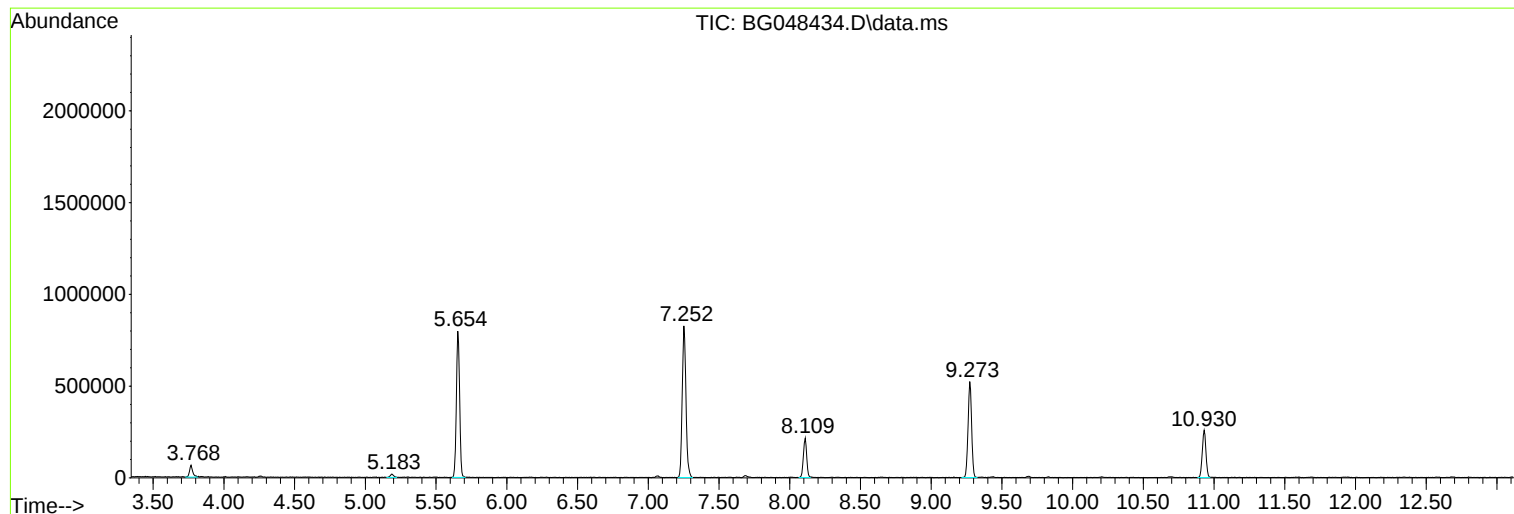
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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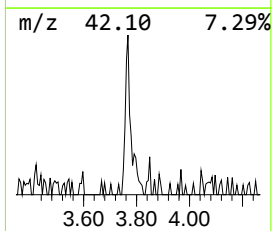
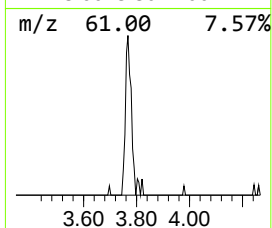
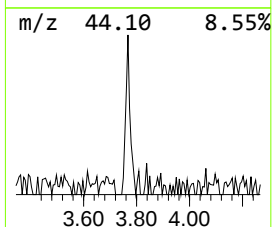
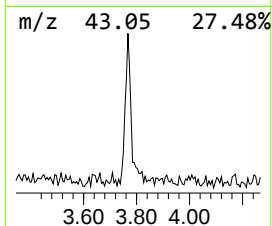
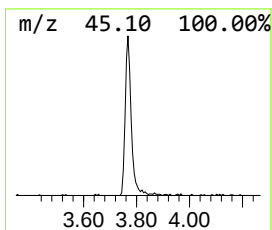
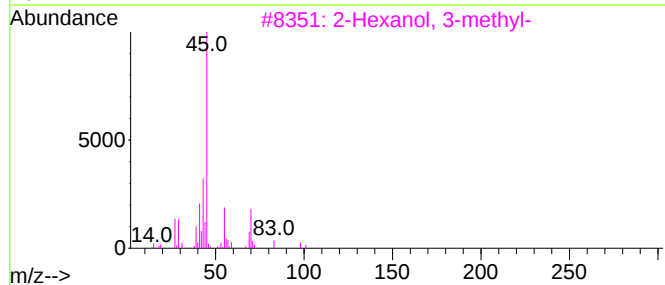
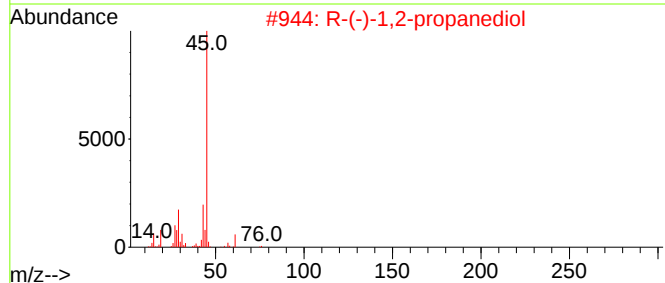
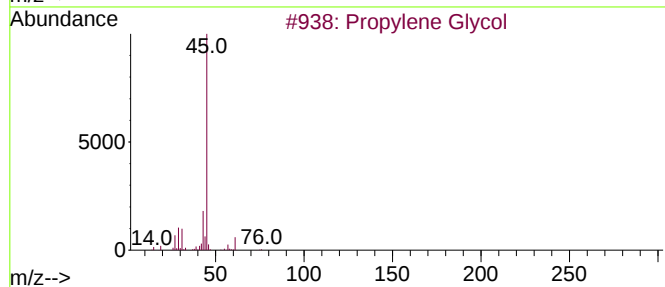
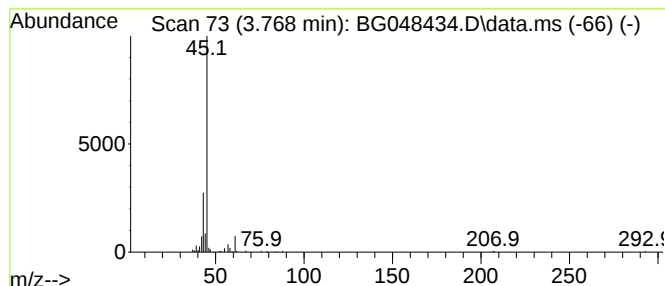
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.768	5.85 ng	101289	1,4-Dichlorobenzene-d4	8.109

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	80
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3			2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	56
4			Hexane, 1-methoxy-	116	C7H16O	004747-07-3	40
5			3-Ethyl-2-pentanol	116	C7H16O	000609-27-8	40



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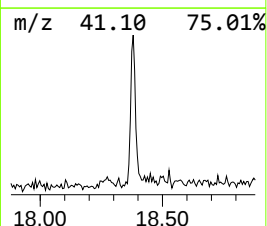
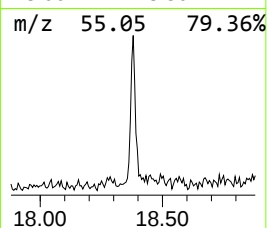
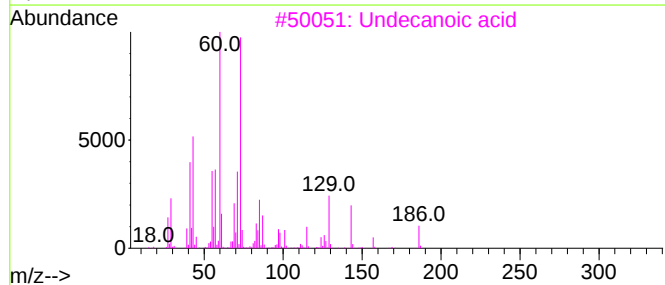
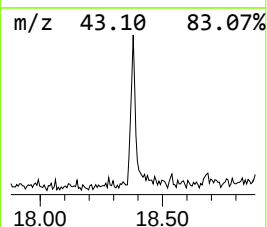
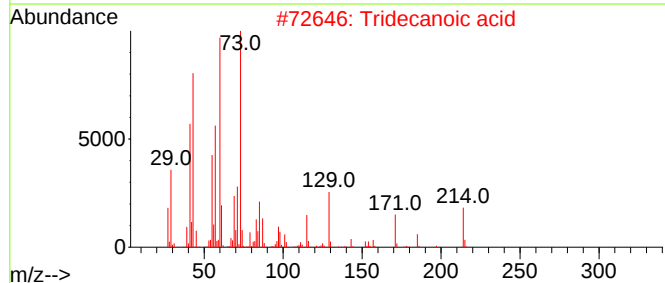
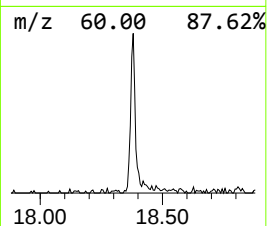
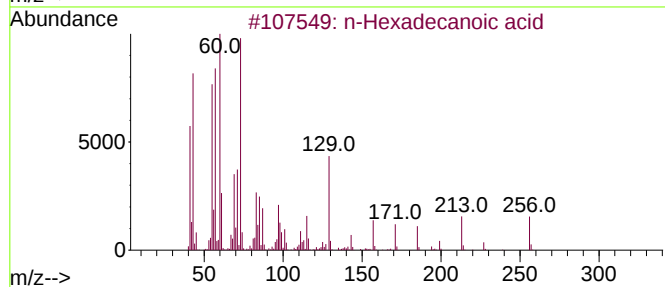
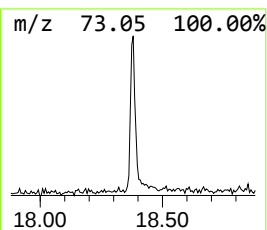
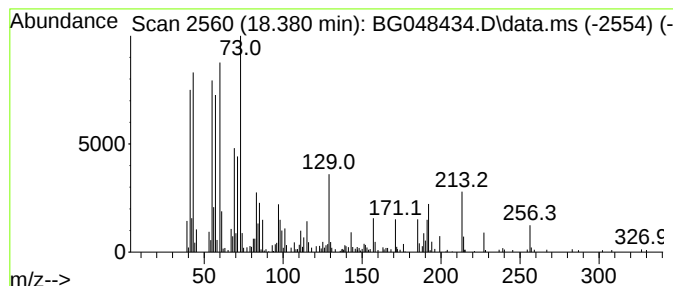
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.380	6.60 ng	289512	Phenanthrene-d10	17.499

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	83
3			Undecanoic acid	186	C11H22O2	000112-37-8	68
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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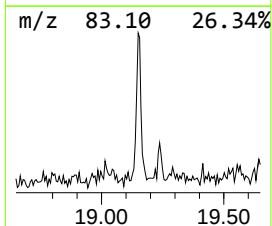
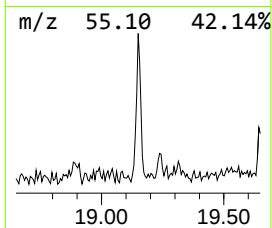
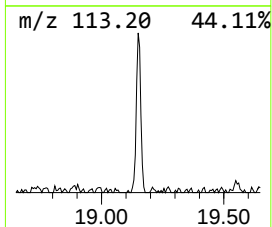
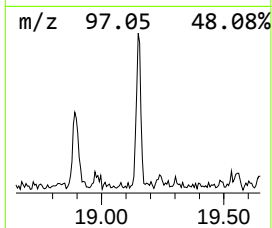
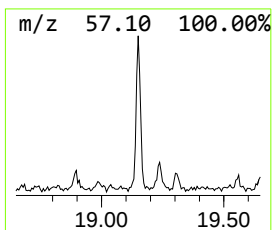
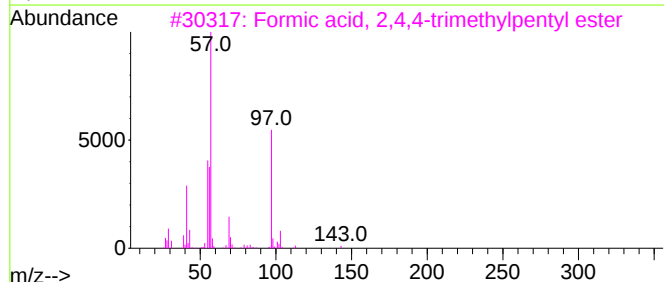
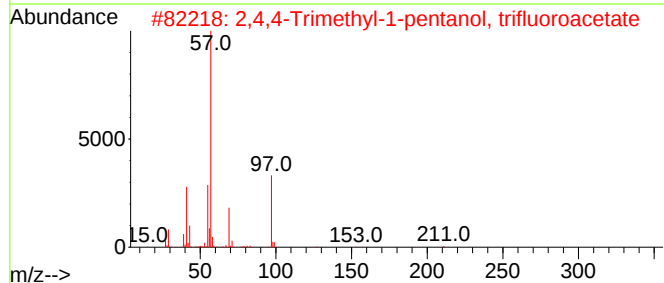
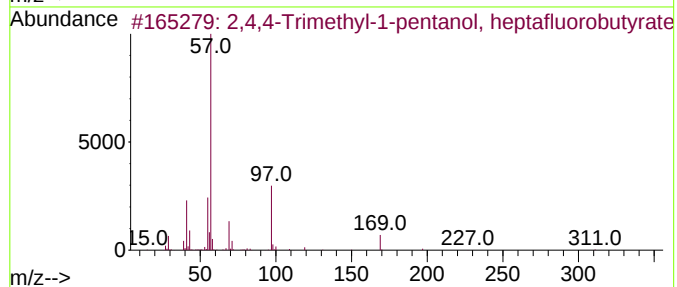
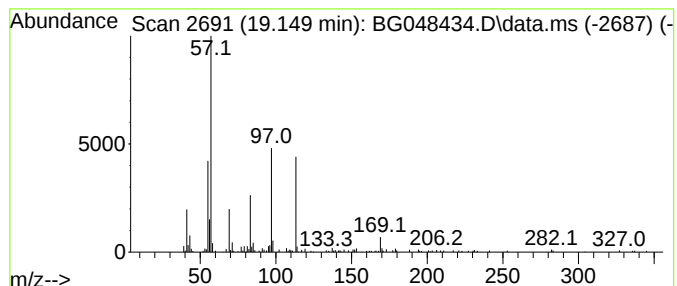
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Peak Number 3 unknown19.150 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.150	2.93 ng	128600	Phenanthrene-d10	17.499

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	35		
2	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	27		
3	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	27		
4	Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	25		
5	1H-Pyrrole-2,5-dione	97	C4H3NO2	000541-59-3	14		



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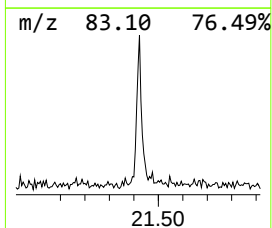
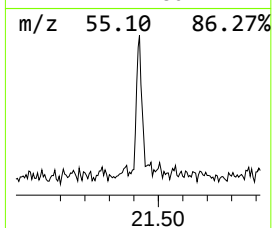
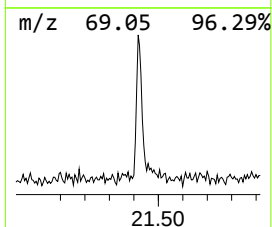
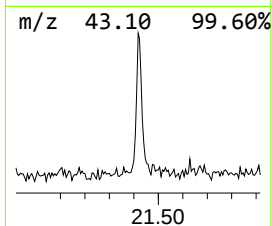
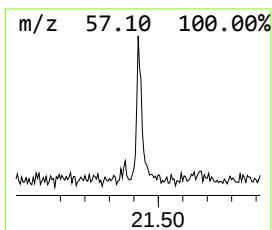
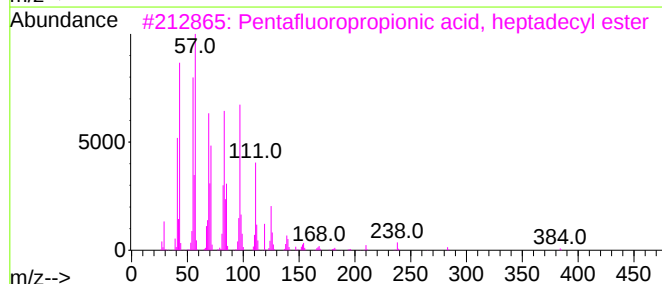
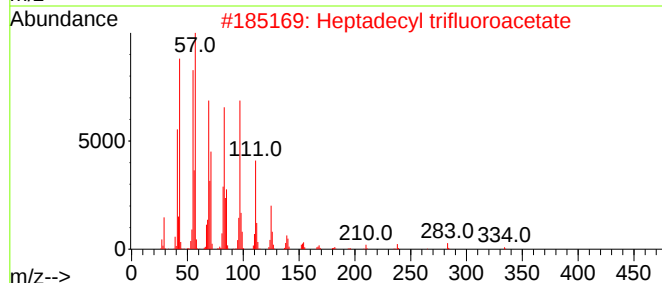
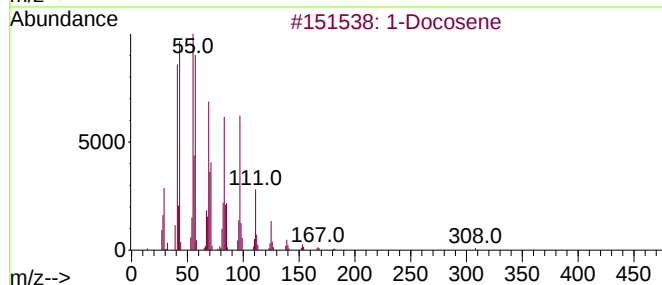
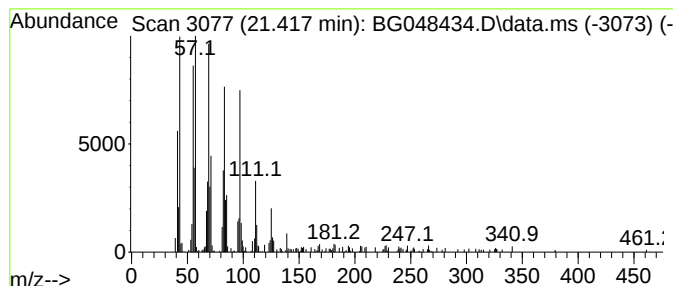
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Peak Number 4 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.417	5.21 ng	297570	Chrysene-d12	21.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	99
2	Heptadecyl trifluoroacetate			352	C19H35F3O2	1000351-87-0	90
3	Pentafluoropropionic acid, hepta...			402	C20H35F5O2	959218-78-1	90
4	n-Tetracosanol-1			354	C24H50O	000506-51-4	89
5	Behenic alcohol			326	C22H46O	000661-19-8	89



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propylene Glycol	3.768	5.8	ng	101289	1	8.109	346500	20.0
n-Hexadecanoic ...	18.380	6.6	ng	289512	4	17.499	877548	20.0
unknown19.150	19.150	2.9	ng	128600	4	17.499	877548	20.0
1-Docosene	21.417	5.2	ng	297570	5	21.793	1141580	20.0