

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
 Data File : BM028550.D
 Acq On : 26 Jan 2021 20:46
 Operator : CG/JU
 Sample : M1220-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP1-C

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-BM012021.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028550.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	309	314	326	rBB	28616	42080	4.65%	0.695%
2	5.516	389	396	403	rBV	380793	547722	60.59%	9.041%
3	6.951	633	640	645	rBB2	6952	9472	1.05%	0.156%
4	7.146	663	673	686	rBB	359591	594964	65.81%	9.821%
5	7.628	751	755	760	rVB	15062	20883	2.31%	0.345%
6	7.987	807	816	823	rBV	119964	186406	20.62%	3.077%
7	8.628	921	925	933	rBB4	6308	9728	1.08%	0.161%
8	9.163	1009	1016	1023	rBV	237926	380270	42.06%	6.277%
9	10.804	1288	1295	1308	rVB	156318	256639	28.39%	4.236%
10	13.257	1705	1712	1722	rVB	549893	769809	85.15%	12.707%
11	14.080	1848	1852	1859	rVB	14794	20508	2.27%	0.339%
12	14.633	1940	1946	1954	rVB	212824	298586	33.03%	4.929%
13	16.110	2192	2197	2204	rBV	376013	507232	56.11%	8.373%
14	17.362	2404	2410	2415	rBV	222583	315276	34.87%	5.204%
15	18.233	2553	2558	2563	rBV	46319	65705	7.27%	1.085%
16	19.398	2752	2756	2760	rVB	7625	11341	1.25%	0.187%
17	19.498	2769	2773	2780	rBV2	16778	24692	2.73%	0.408%
18	19.762	2814	2818	2824	rBV2	15650	24154	2.67%	0.399%
19	19.951	2845	2850	2856	rBV	706914	904036	100.00%	14.922%
20	20.221	2893	2896	2899	rBV4	10308	14993	1.66%	0.247%
21	21.192	3057	3061	3071	rBV	174064	234297	25.92%	3.867%
22	21.492	3107	3112	3118	rBV	278677	367252	40.62%	6.062%
23	22.086	3210	3213	3219	rVB2	70405	96238	10.65%	1.589%
24	23.762	3493	3498	3507	rVB	191148	356026	39.38%	5.877%

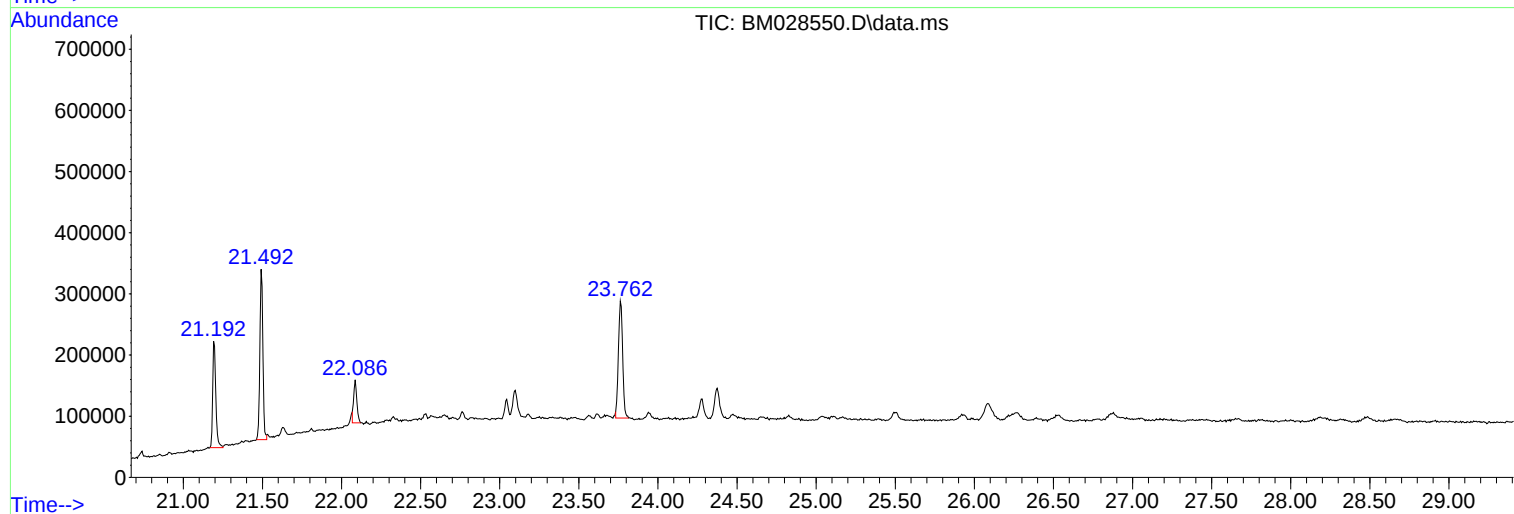
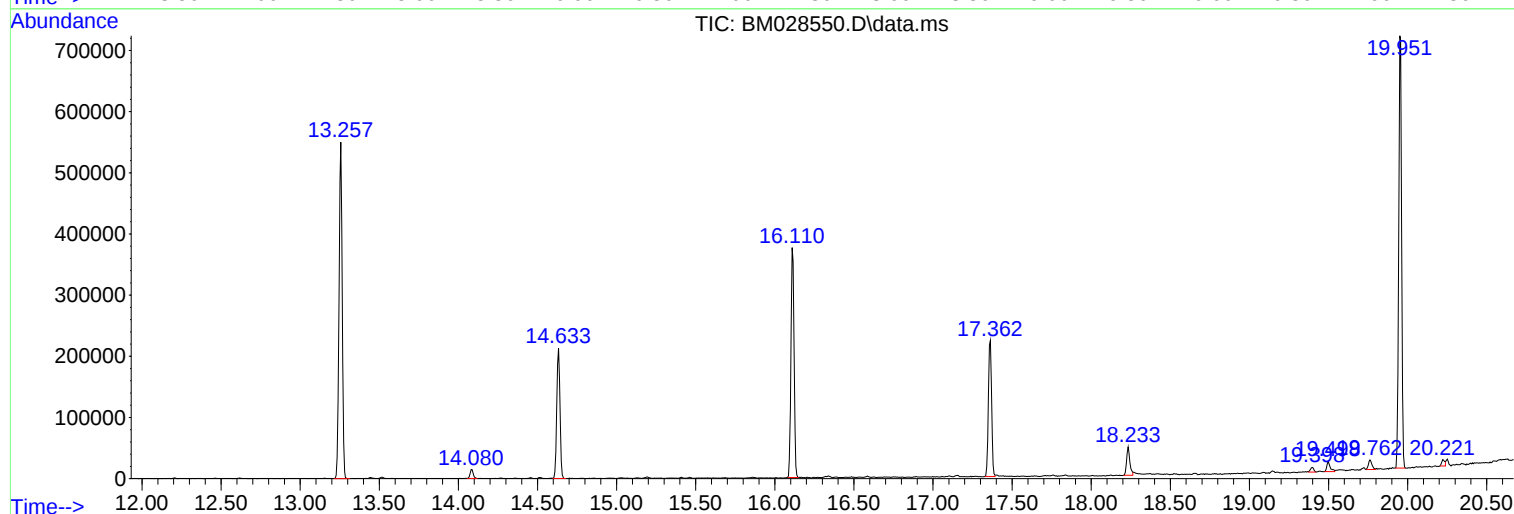
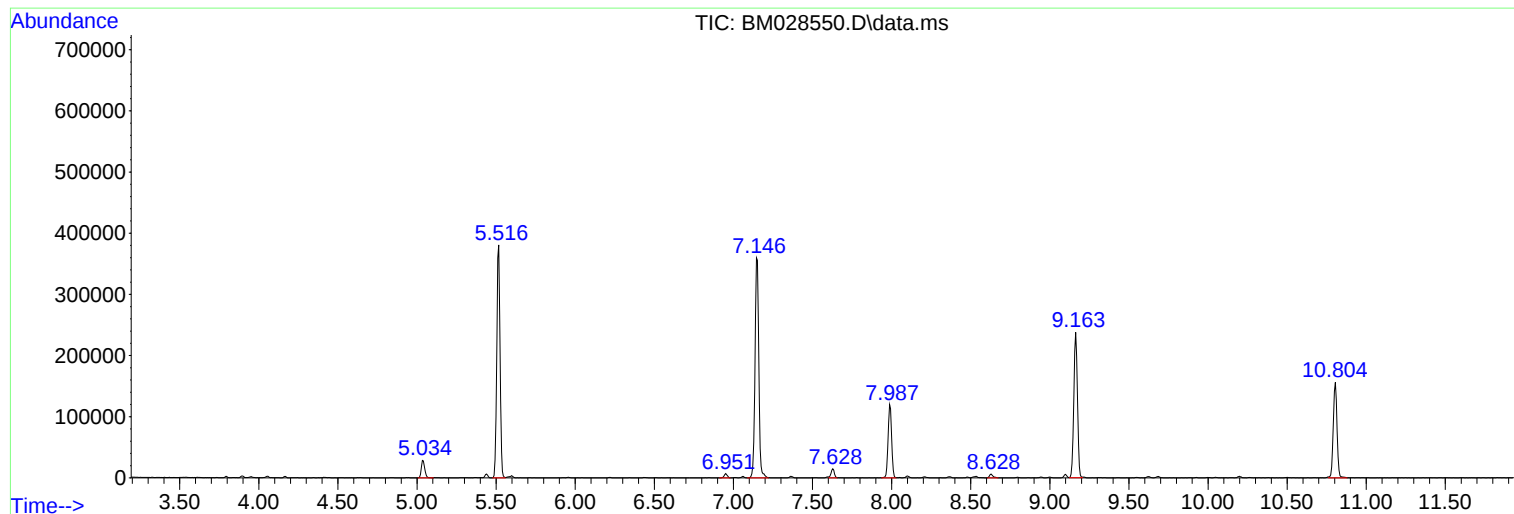
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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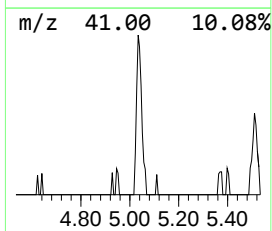
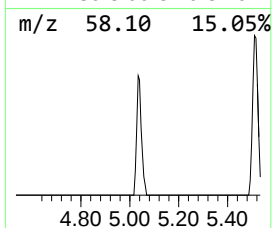
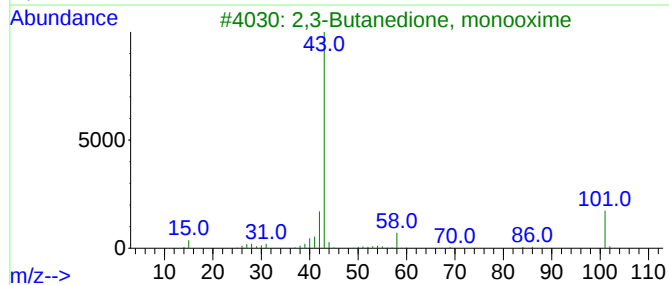
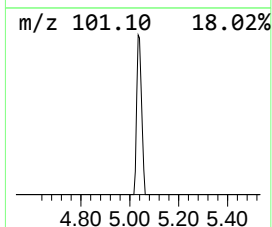
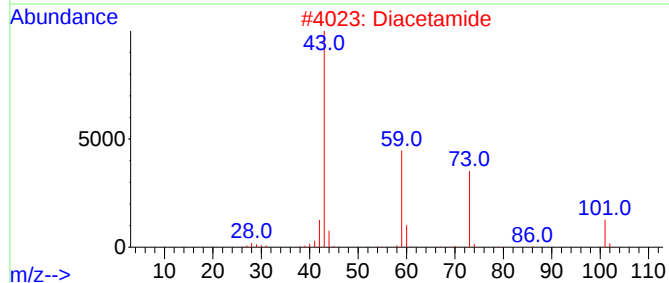
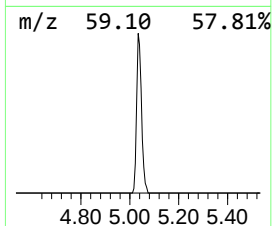
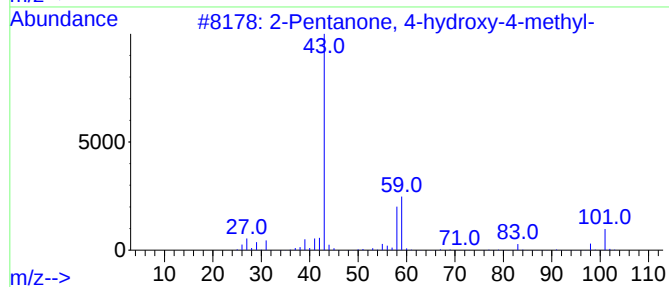
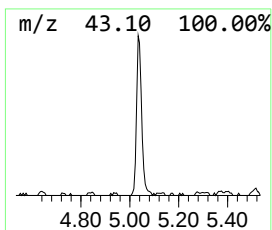
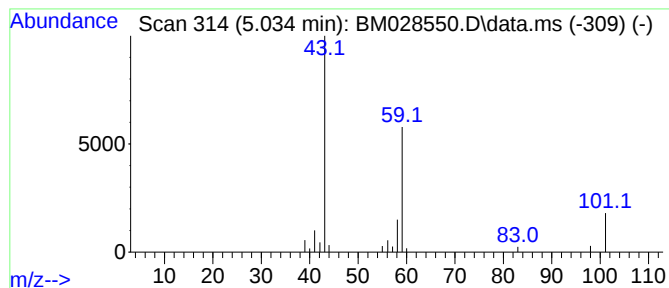
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	4.51 ng	42080	1,4-Dichlorobenzene-d4	7.987

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Diacetamide	101	C4H7NO2	000625-77-4	9		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	3-Hexanol	102	C6H14O	000623-37-0	9		
5	3-Octanol	130	C8H18O	000589-98-0	9		



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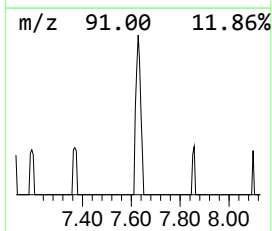
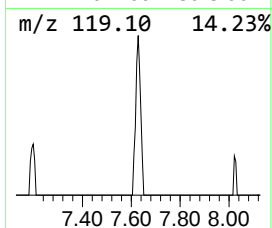
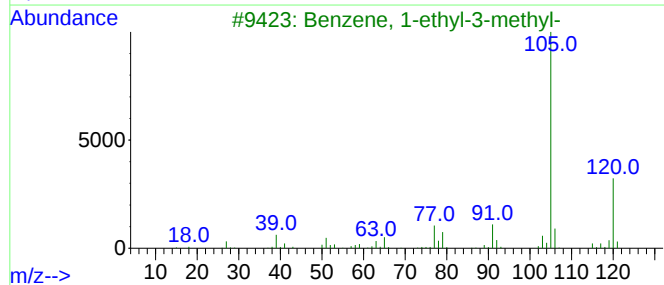
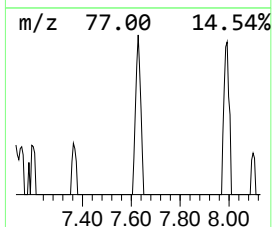
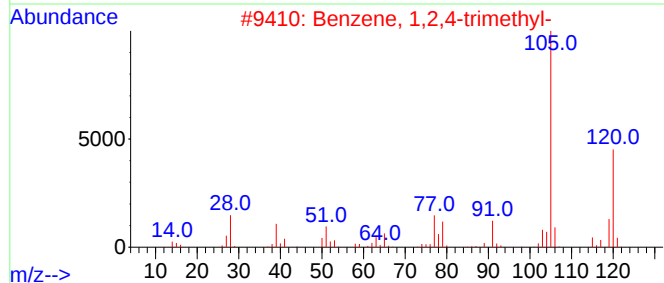
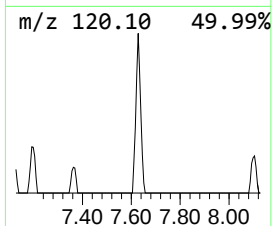
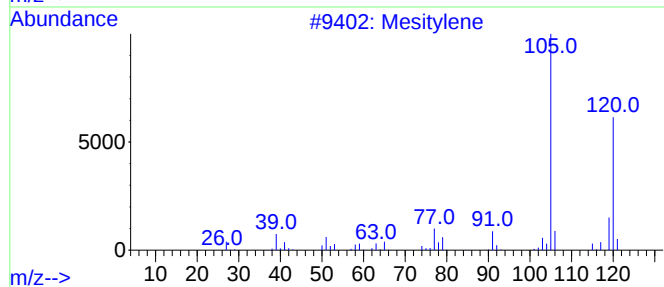
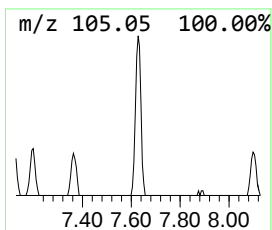
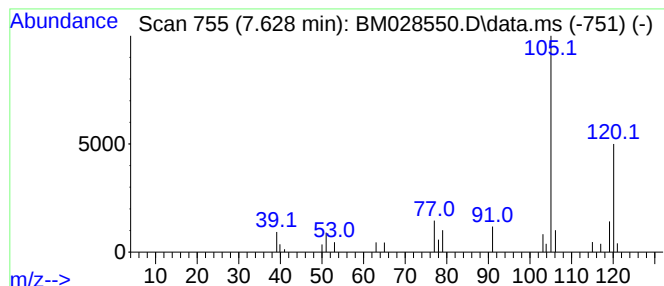
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Peak Number 2 Mesitylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.628	2.24 ng	20883	1,4-Dichlorobenzene-d4	7.987

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Mesitylene	120	C9H12	000108-67-8	94
2		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



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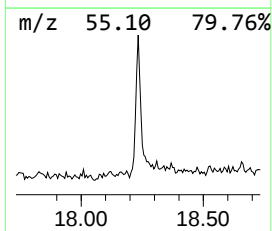
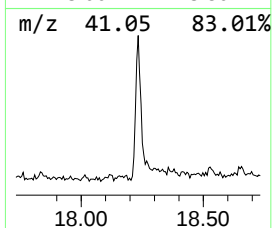
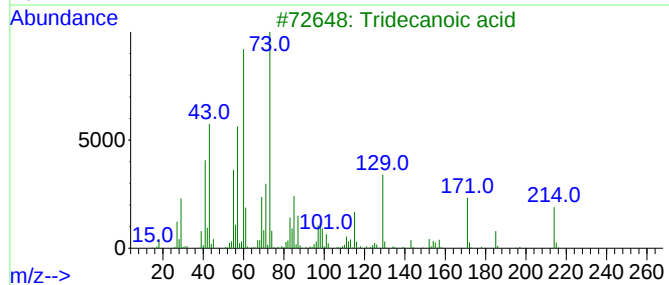
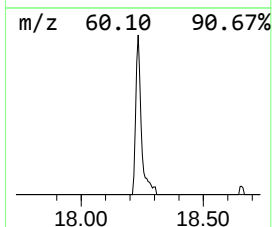
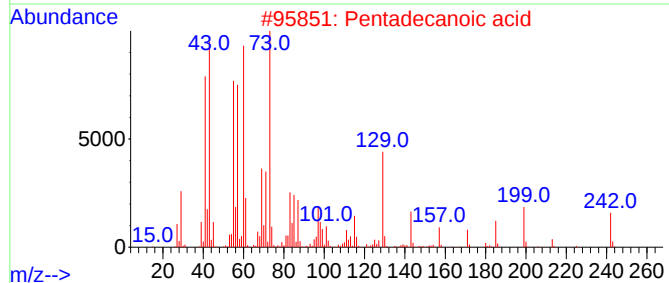
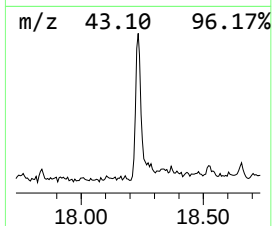
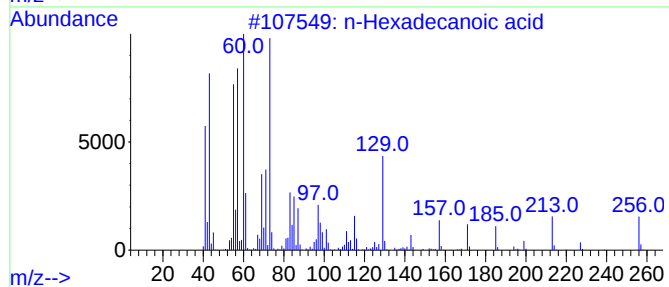
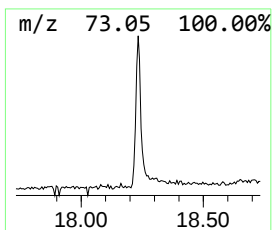
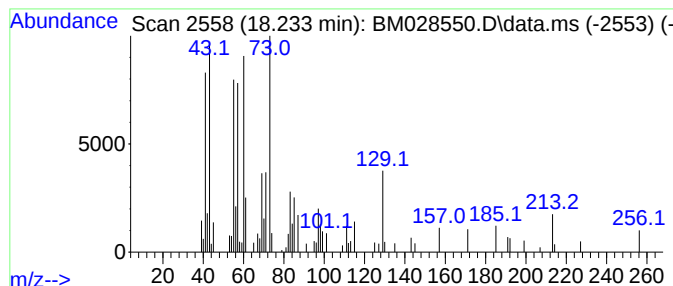
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	4.17 ng	65705	Phenanthrene-d10	17.363

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			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Dodecanoic acid	200	C12H24O2	000143-07-7	43



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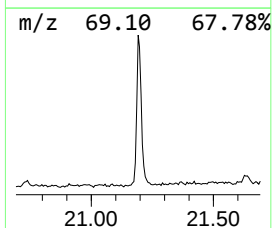
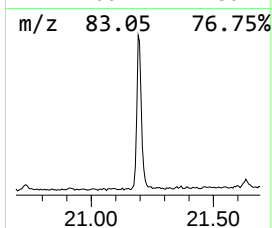
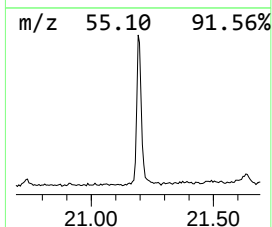
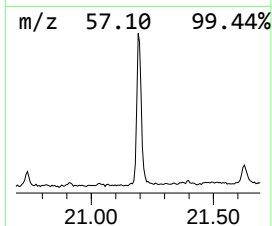
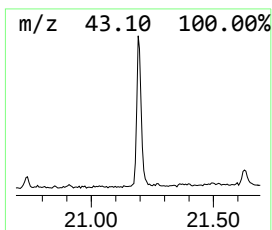
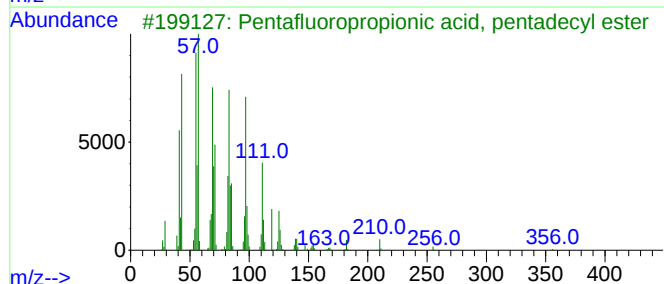
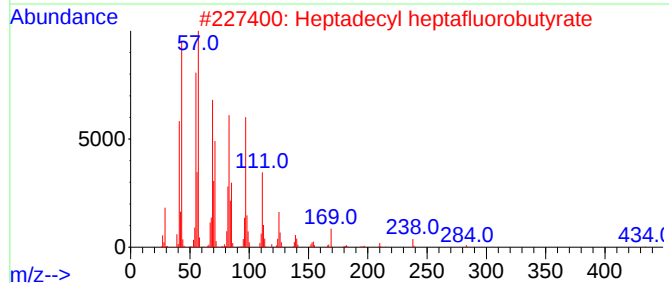
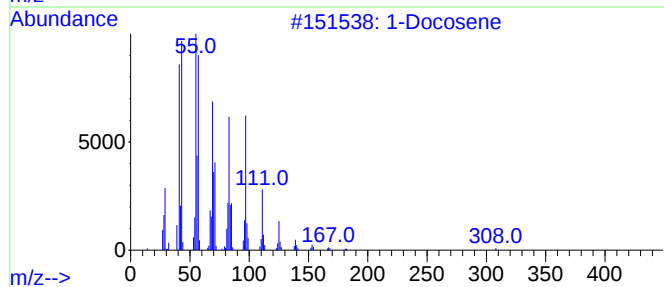
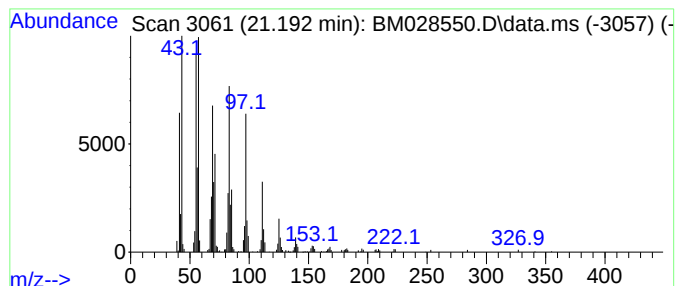
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Peak Number 4 1-Docosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.192	12.76 ng	234297	Chrysene-d12	21.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	95
2	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	94
3	Pentafluoropropionic acid, penta...			374	C18H31F5O2	959092-08-1	94
4	Heptafluorobutyric acid, pentade...			424	C19H31F7O2	959261-23-5	94
5	Trifluoroacetic acid, pentadecyl...			324	C17H31F3O2	959010-23-2	94



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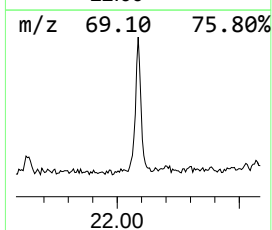
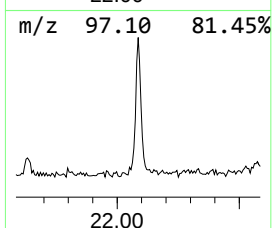
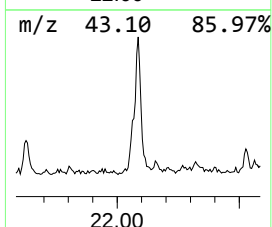
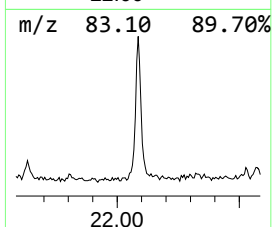
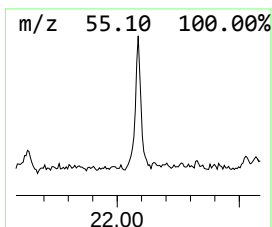
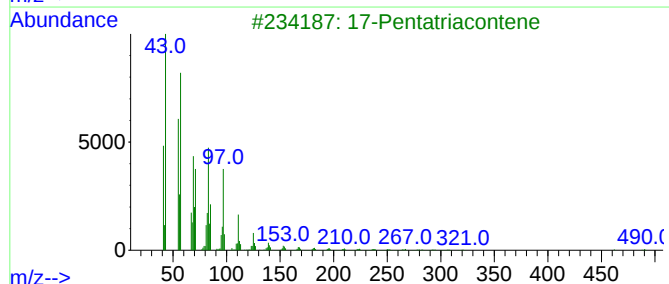
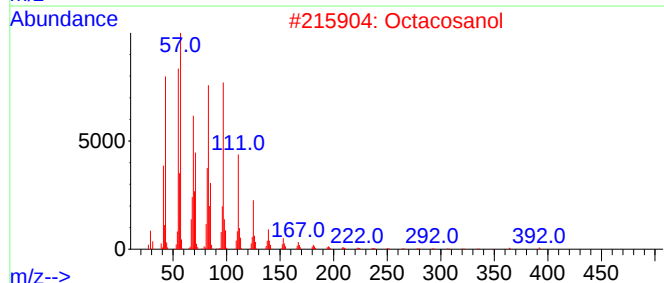
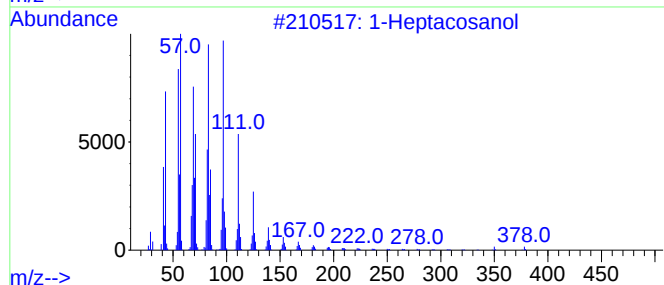
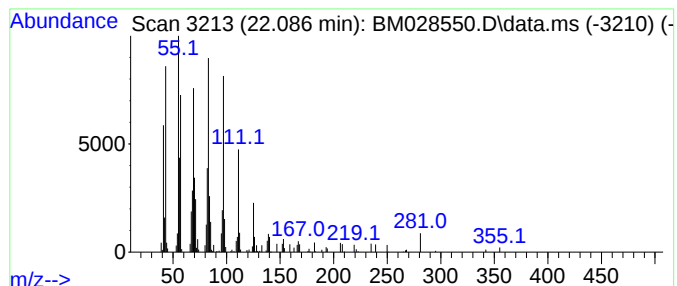
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Peak Number 5 1-Heptacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.086	5.24 ng	96238	Chrysene-d12	21.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	91
2			Octacosanol	410	C28H58O	000557-61-9	90
3			17-Pentatriacontene	491	C35H70	006971-40-0	87
4			1-Hexadecanol	242	C16H34O	036653-82-4	81
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	74



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.034	4.5	ng	42080	1	7.987	186406	20.0
Mesitylene	7.628	2.2	ng	20883	1	7.987	186406	20.0
n-Hexadecanoic ...	18.233	4.2	ng	65705	4	17.363	315276	20.0
1-Docosene	21.192	12.8	ng	234297	5	21.492	367252	20.0
1-Heptacosanol	22.086	5.2	ng	96238	5	21.492	367252	20.0