

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022723\
 Data File : BF132556.D
 Acq On : 27 Feb 2023 17:04
 Operator : CG\JU
 Sample : 01701-02
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-19-SB02

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-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132556.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.637	302	306	310	rBV	47972	53038	1.43%	0.193%
2	5.243	403	409	423	rVB	1627439	2092036	56.30%	7.623%
3	5.631	471	475	479	rBV	3293970	3327431	89.55%	12.124%
4	6.019	537	541	548	rBV	92516	76746	2.07%	0.280%
5	6.631	640	645	648	rBV	3517671	3389200	91.22%	12.349%
6	7.001	705	708	712	rBV	1045460	839417	22.59%	3.059%
7	7.566	799	804	807	rBV	2374882	2243374	60.38%	8.174%
8	8.289	923	927	930	rBV	1378621	1054432	28.38%	3.842%
9	9.366	1106	1110	1113	rBV	4512729	3715554	100.00%	13.538%
10	10.048	1223	1226	1230	rBV	1358946	1122984	30.22%	4.092%
11	10.766	1344	1348	1351	rBV	1396948	1122704	30.22%	4.091%
12	10.842	1357	1361	1365	rBV	2319055	2131724	57.37%	7.767%
13	11.072	1397	1400	1408	rVB	143629	124620	3.35%	0.454%
14	11.542	1477	1480	1484	rBV	1056497	968047	26.05%	3.527%
15	12.054	1564	1567	1580	rBV	255955	306799	8.26%	1.118%
16	12.848	1698	1702	1709	rBV	43951	60452	1.63%	0.220%
17	13.136	1747	1751	1754	rBV	3354661	2948723	79.36%	10.744%
18	14.030	1899	1903	1914	rBV	178692	363196	9.78%	1.323%
19	14.201	1928	1932	1936	rBV	881989	839549	22.60%	3.059%
20	14.660	2007	2010	2014	rBV3	33660	43040	1.16%	0.157%
21	15.754	2191	2196	2201	rBV2	468997	621500	16.73%	2.265%

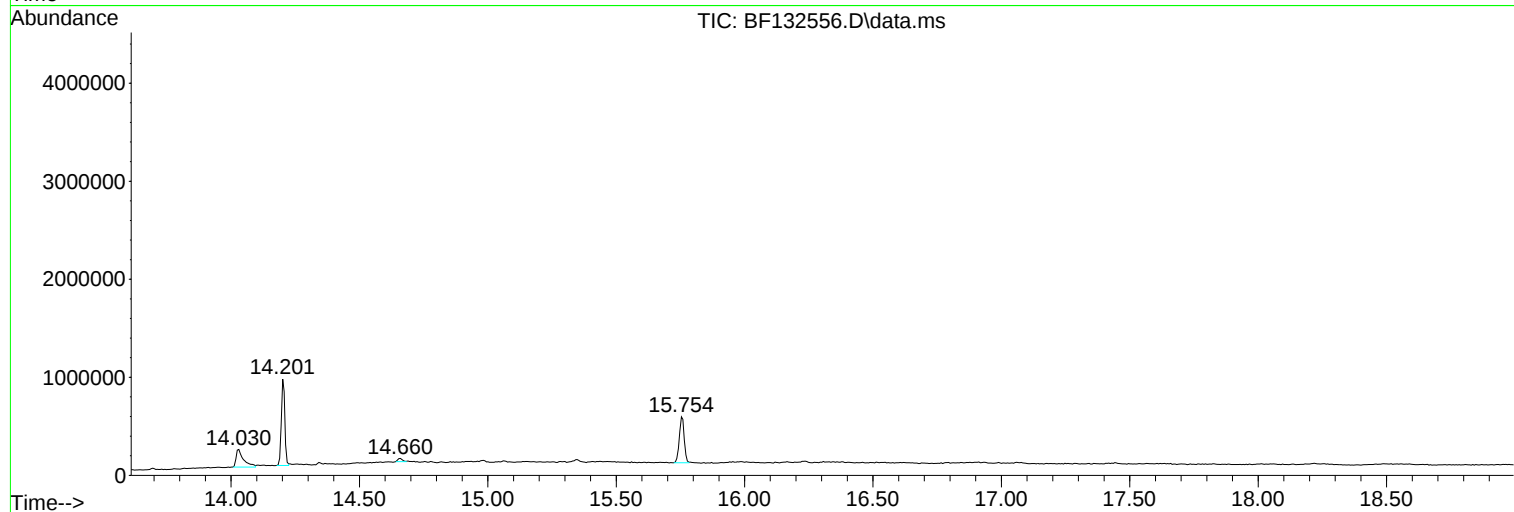
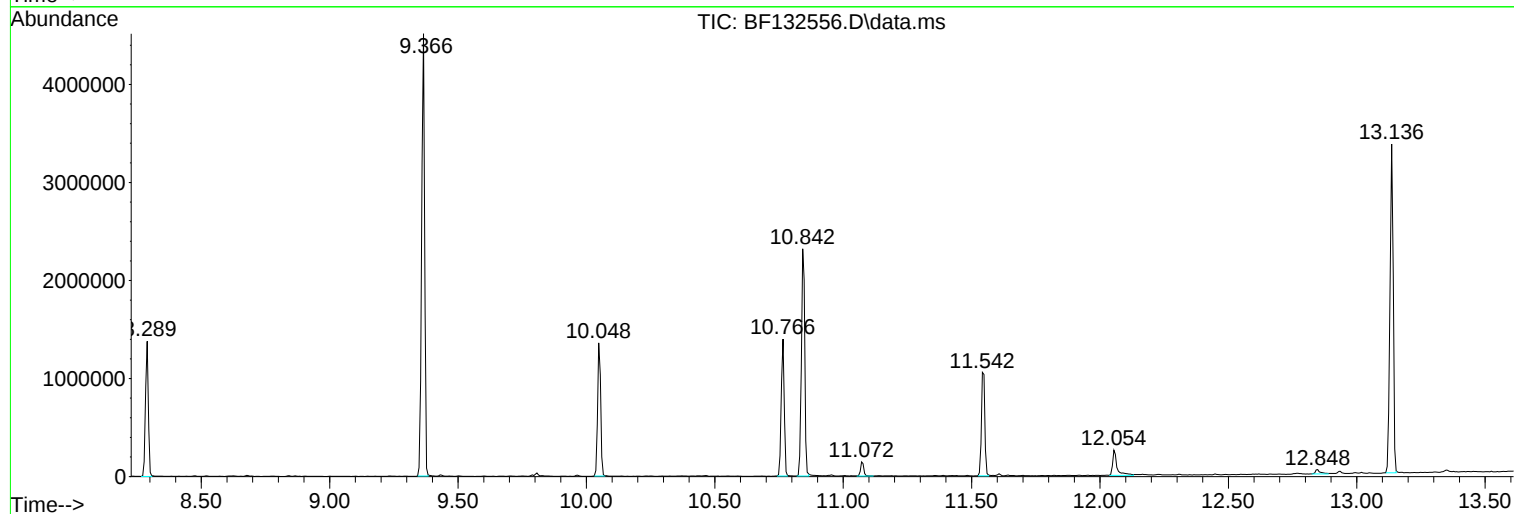
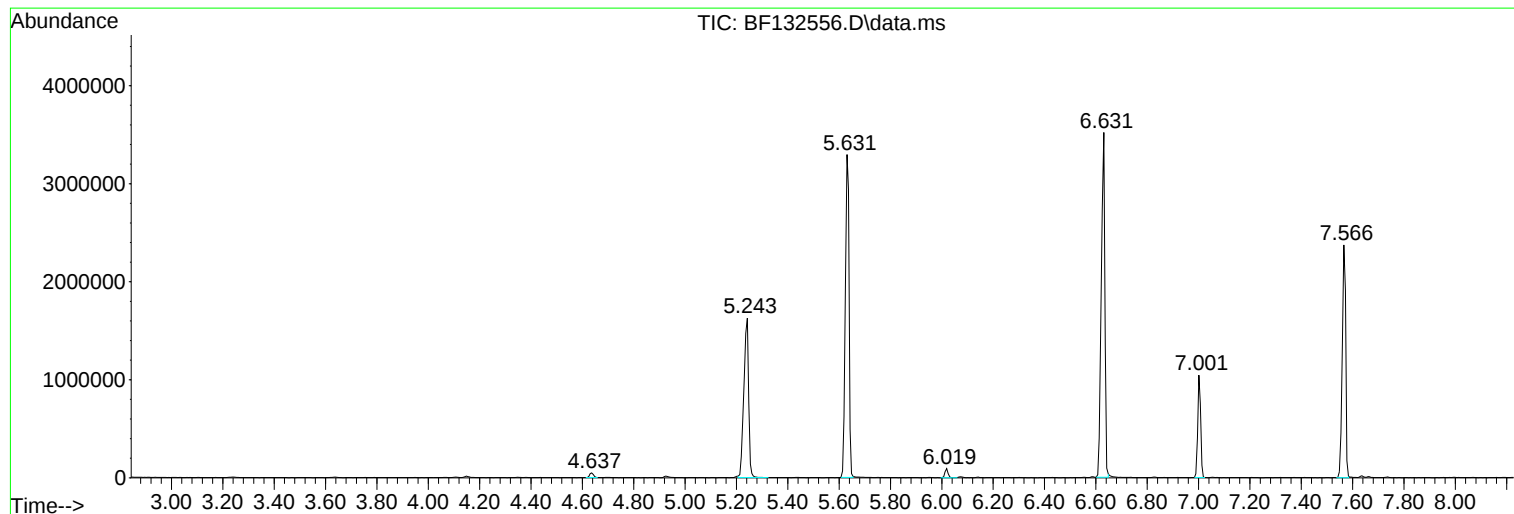
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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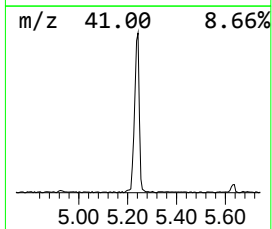
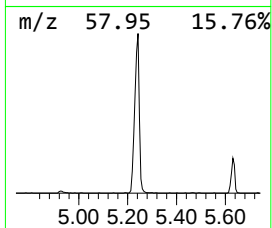
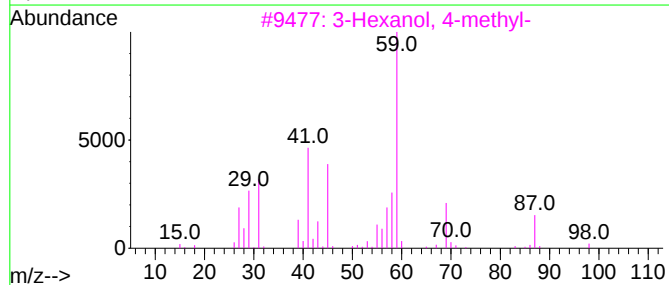
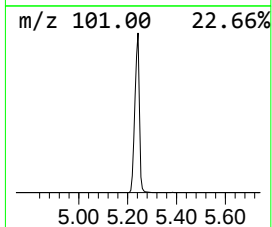
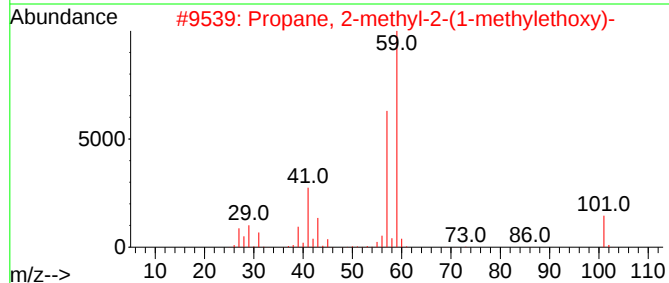
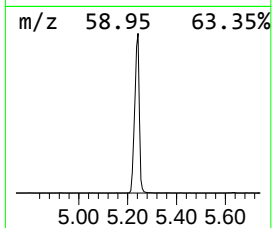
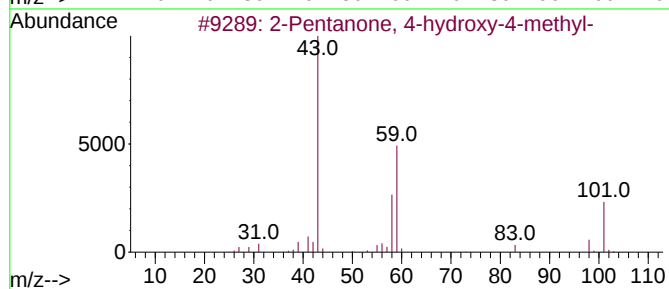
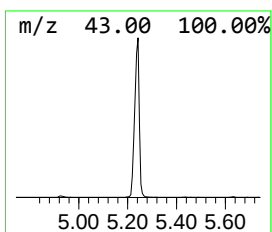
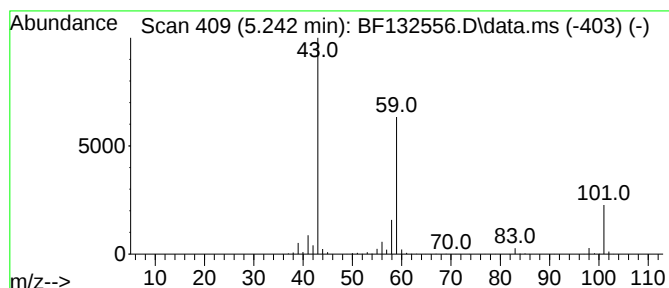
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.242	49.84 ng	2092040	1,4-Dichlorobenzene-d4	7.001

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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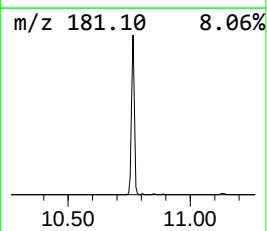
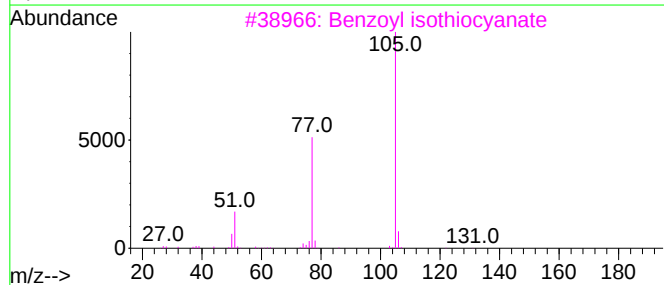
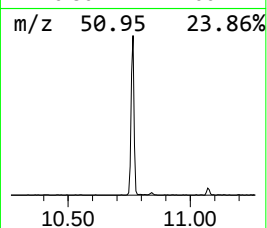
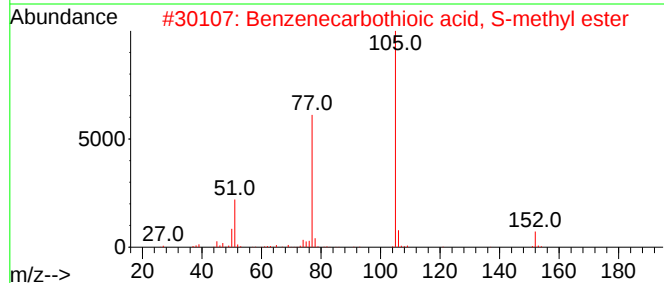
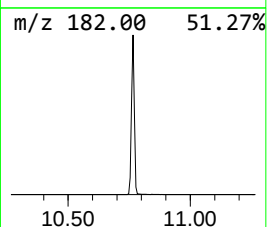
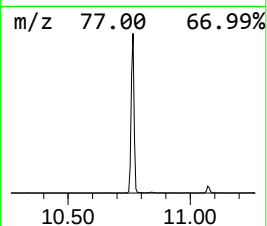
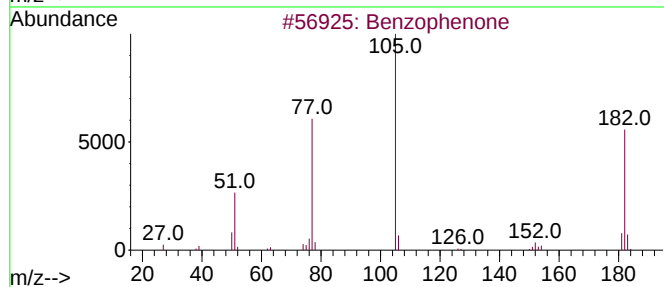
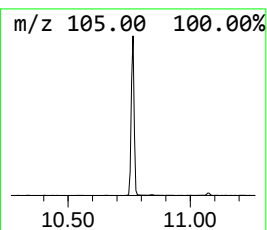
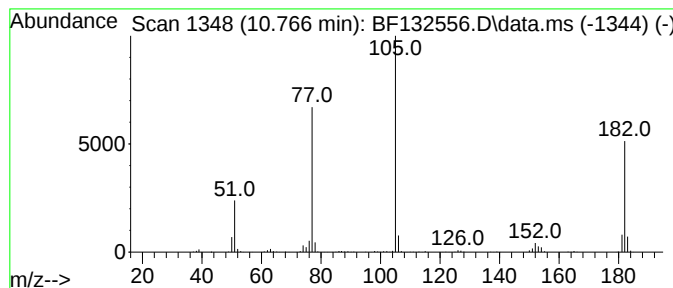
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.766	20.00 ng	1122700	Acenaphthene-d10	10.048

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
4			Vinyl benzoate	148	C9H8O2	000769-78-8	47
5			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47



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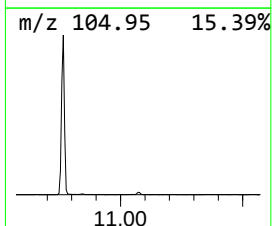
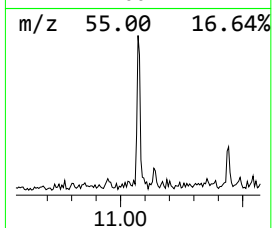
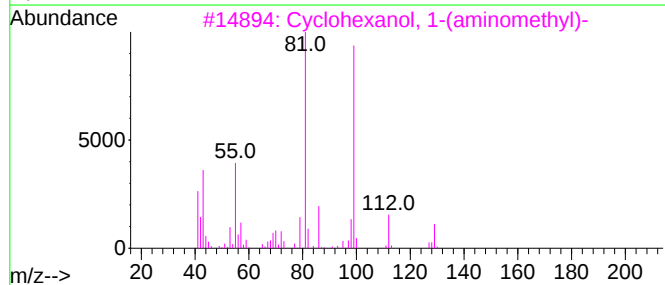
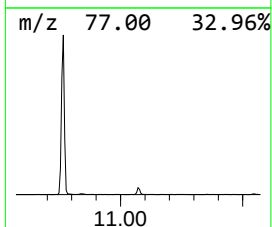
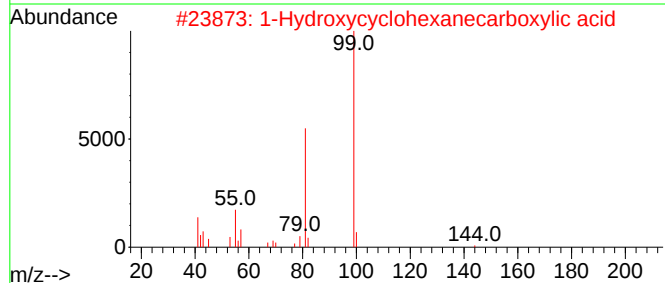
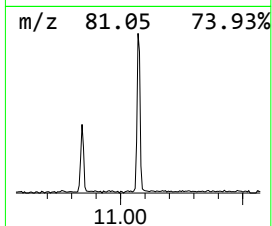
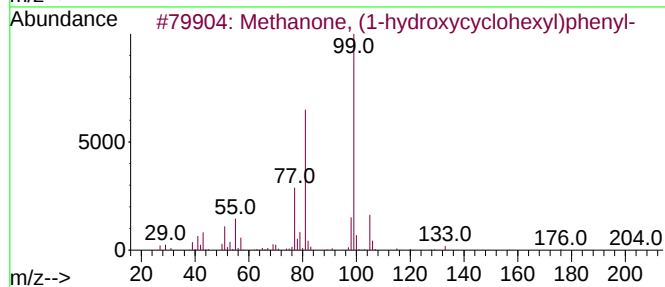
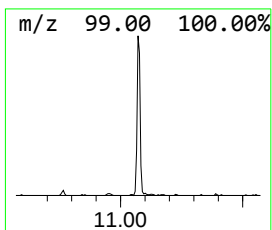
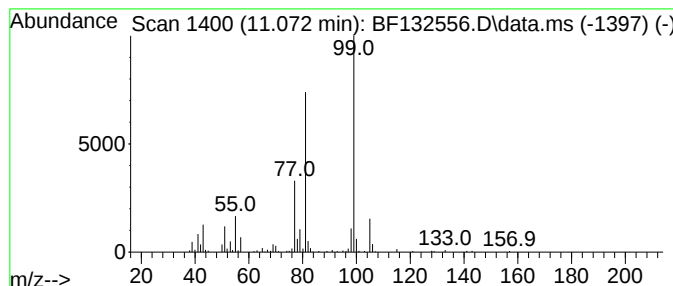
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Peak Number 3 Methanone, (1-hydroxycyclohexyl) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.072	2.57 ng	124620	Phenanthrene-d10	11.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	90
2			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	59
3			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	50
4			Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	45
5			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	42



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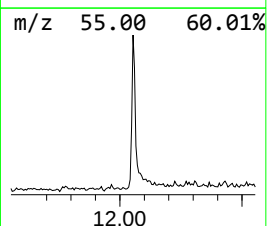
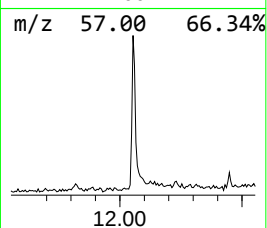
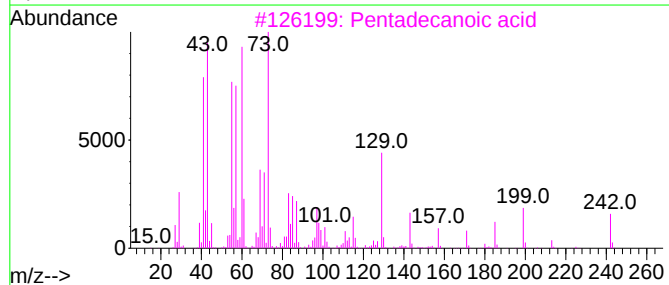
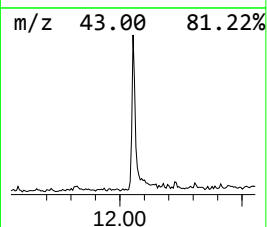
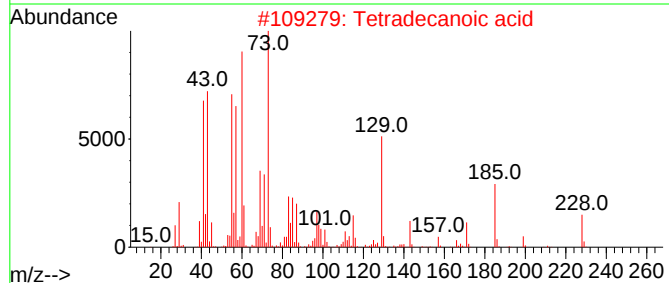
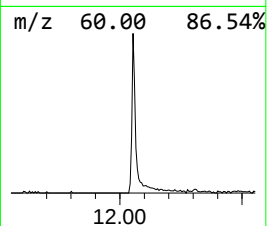
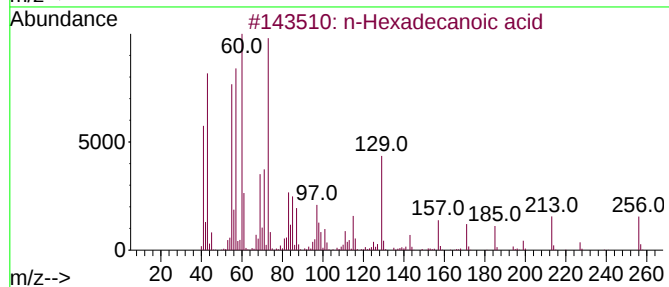
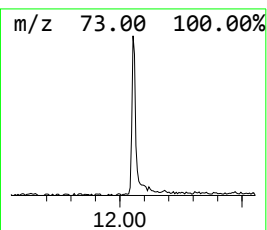
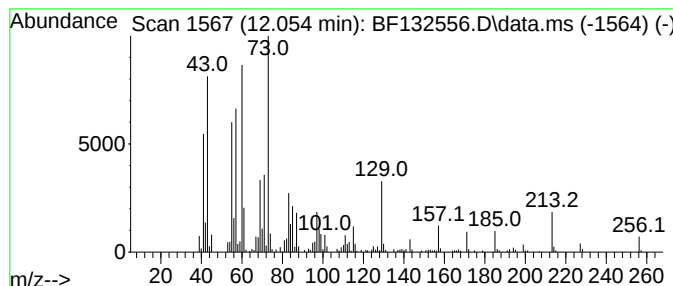
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.054	6.34 ng	306799	Phenanthrene-d10	11.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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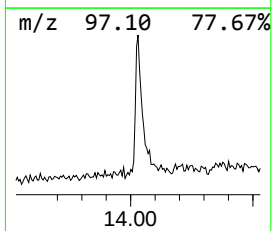
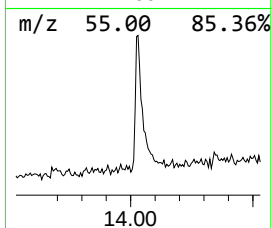
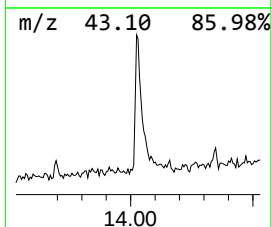
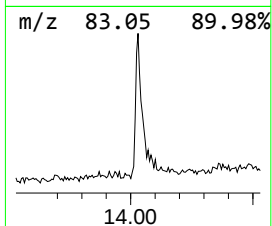
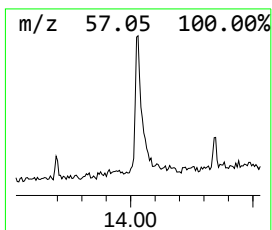
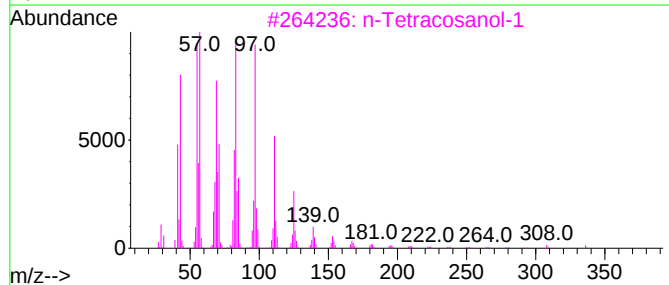
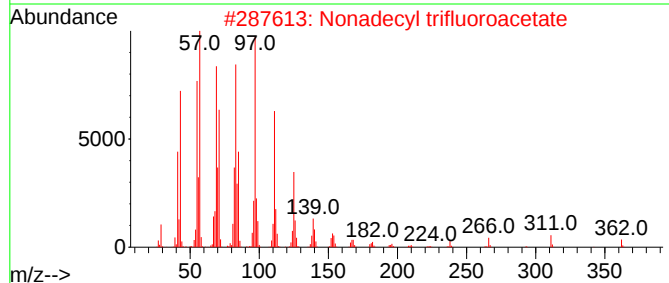
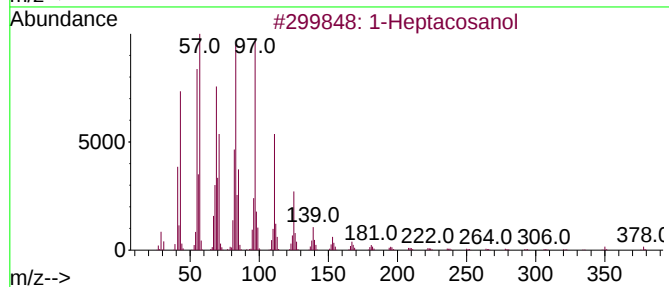
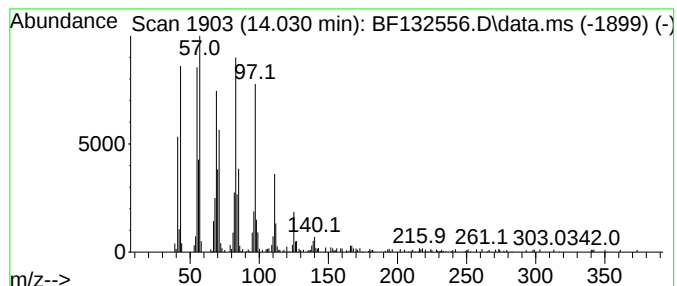
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Peak Number 5 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.030	8.65 ng	363196	Chrysene-d12	14.201

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptacosanol	396	C27H56O	002004-39-9	94
2		Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5		Pentacos-1-ene	350	C25H50	016980-85-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.242	49.8	ng	2092040	1	7.001	839417	20.0
Benzophenone	10.766	20.0	ng	1122700	3	10.048	1122980	20.0
Methanone, (1-h...	11.072	2.6	ng	124620	4	11.548	968047	20.0
n-Hexadecanoic ...	12.054	6.3	ng	306799	4	11.548	968047	20.0
1-Heptacosanol	14.030	8.7	ng	363196	5	14.201	839549	20.0