

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031924\
 Data File : BG060678.D
 Acq On : 19 Mar 2024 11:46
 Operator : MA/JU
 Sample : PB159643BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB159643BL

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-BG031324.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060678.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.323	323	329	337	rBV	100880	156428	1.87%	0.435%
2	5.781	396	407	419	rBV	2299797	3637748	43.43%	10.111%
3	7.408	675	684	692	rBV	1916749	3229888	38.56%	8.977%
4	8.290	827	834	842	rVB	336639	567183	6.77%	1.576%
5	9.488	1029	1038	1050	rBV	1069307	1857375	22.18%	5.162%
6	11.134	1309	1318	1326	rBV	475300	859270	10.26%	2.388%
7	13.542	1721	1728	1736	rBV	2986293	4704917	56.18%	13.077%
8	14.923	1953	1963	1971	rBV	780594	1237241	14.77%	3.439%
9	16.404	2207	2215	2228	rBV	2472111	3810102	45.49%	10.590%
10	17.667	2423	2430	2439	rBV	1157495	1761941	21.04%	4.897%
11	19.900	2805	2810	2814	rBV	171952	212239	2.53%	0.590%
12	20.252	2864	2870	2876	rBV	6244879	8375271	100.00%	23.278%
13	20.940	2983	2987	2995	rBV2	124183	171232	2.04%	0.476%
14	21.986	3158	3165	3173	rBV	1095561	1917679	22.90%	5.330%
15	22.767	3293	3298	3308	rVB2	52979	114230	1.36%	0.317%
16	23.519	3420	3426	3435	rVB2	74410	152118	1.82%	0.423%
17	24.400	3570	3576	3585	rVB3	89487	206960	2.47%	0.575%
18	25.446	3746	3754	3757	rBV3	109360	255753	3.05%	0.711%
19	25.517	3757	3766	3783	rVB	695142	2148857	25.66%	5.972%
20	26.698	3958	3967	3976	rBV4	89655	294425	3.52%	0.818%
21	28.214	4215	4225	4238	rVB2	85981	308817	3.69%	0.858%

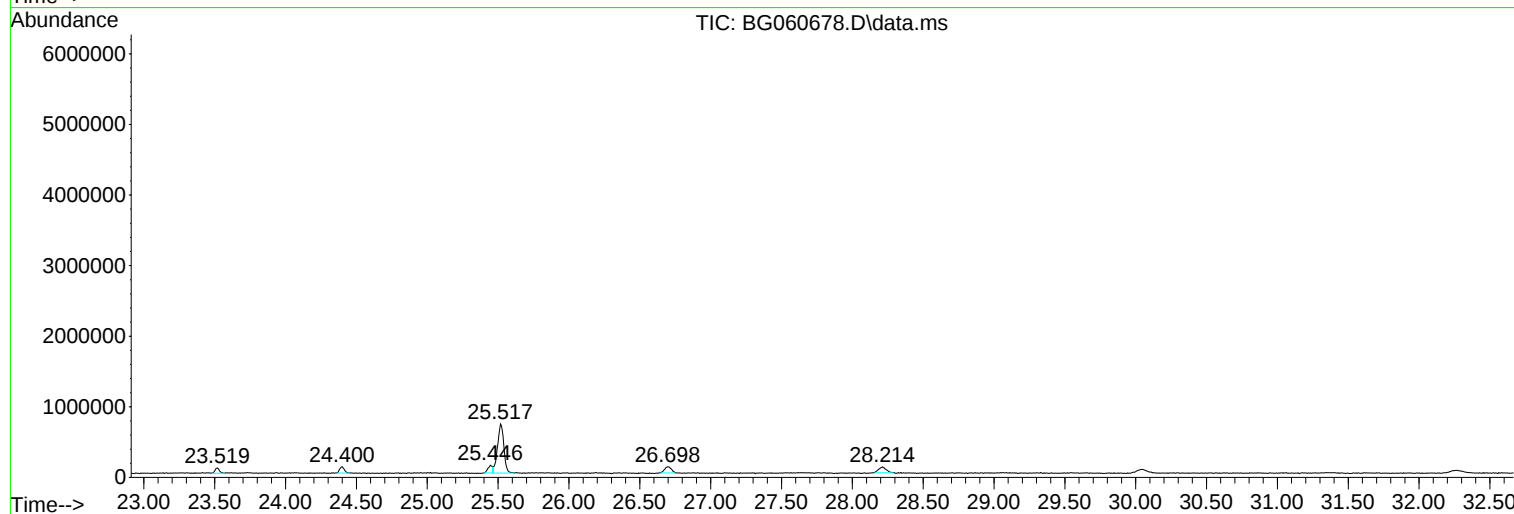
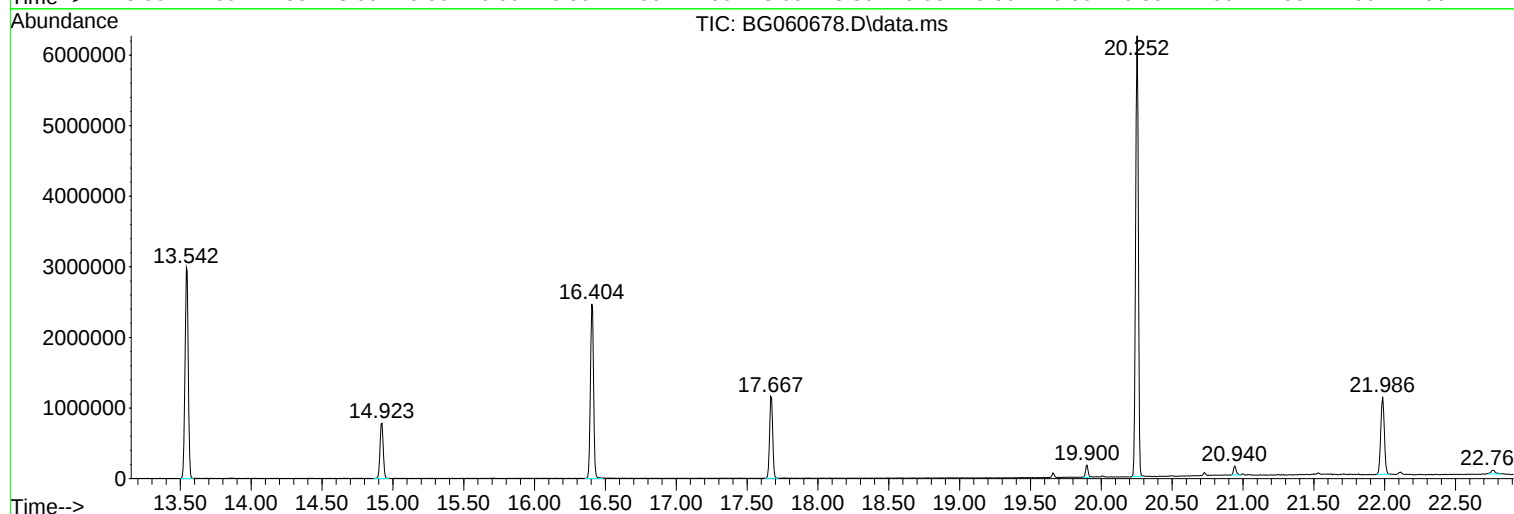
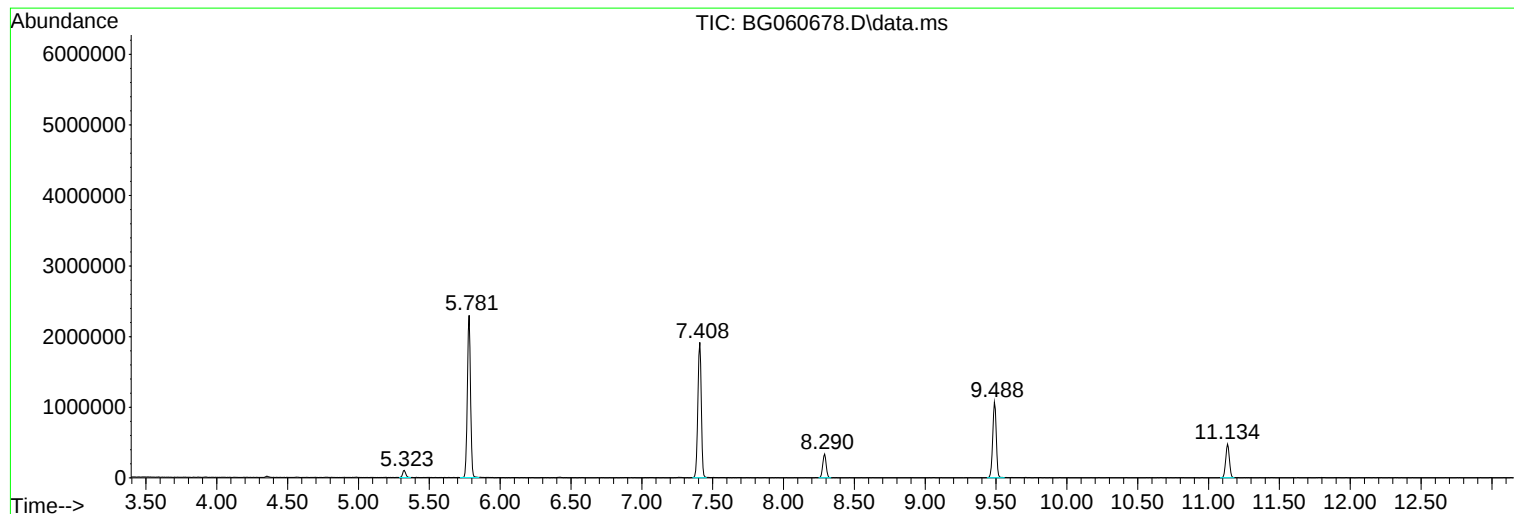
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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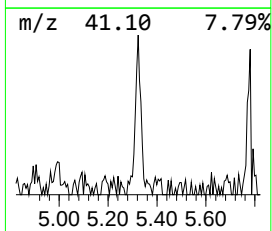
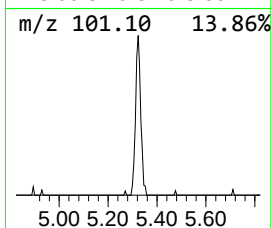
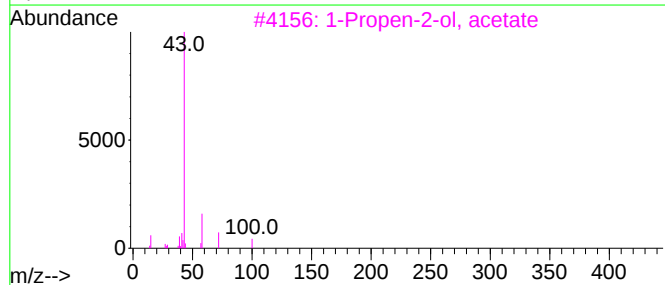
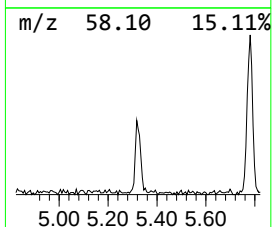
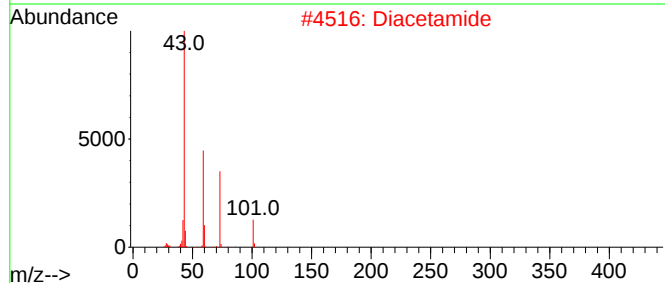
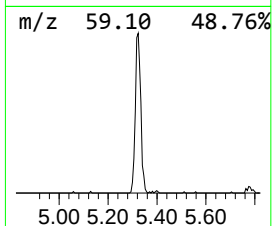
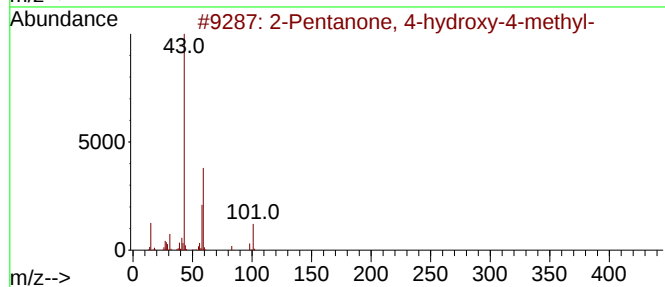
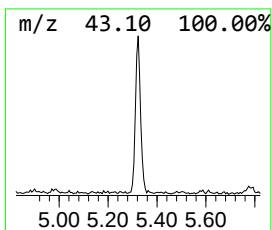
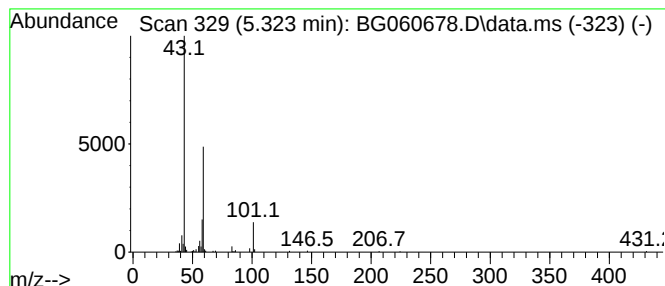
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.323	5.52 ng	156428	1,4-Dichlorobenzene-d4			8.290
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	59
2	Diacetamide		101	C4H7NO2	000625-77-4	9
3	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	9
4	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	9
5	5-Oxohexanenitrile		111	C6H9NO	010412-98-3	9



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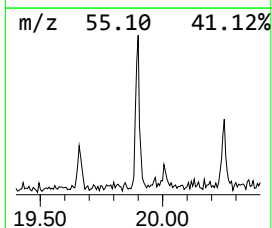
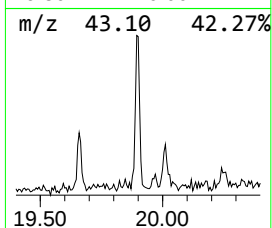
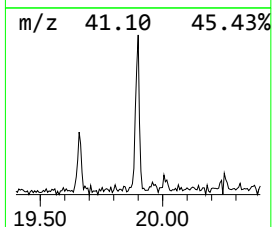
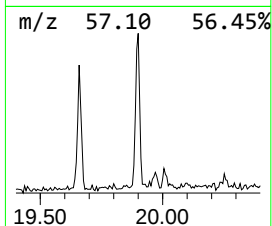
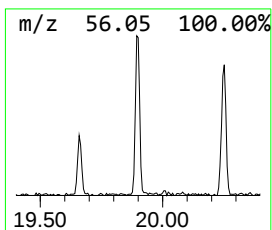
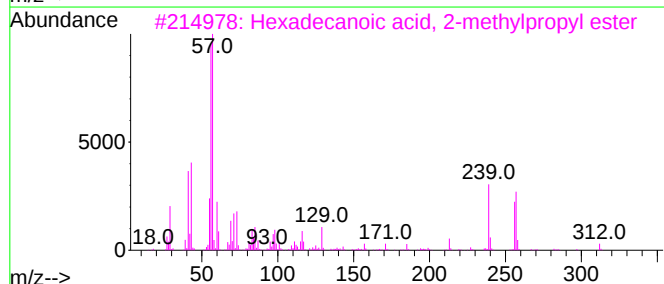
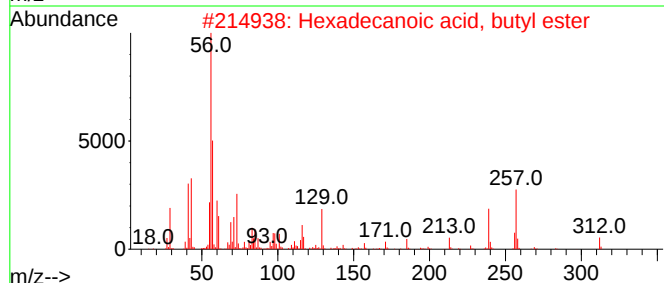
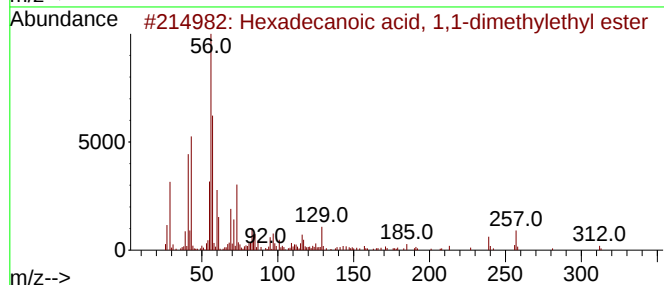
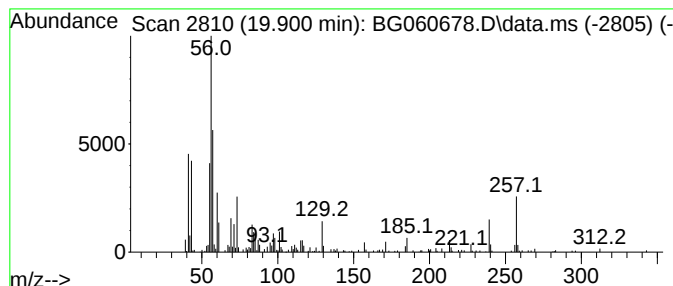
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.900	2.21 ng	212239	Chrysene-d12	21.985

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
2			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	86
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	41
4			1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	38
5			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



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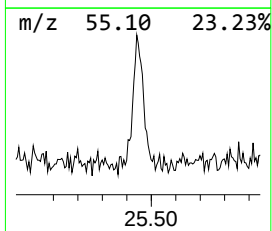
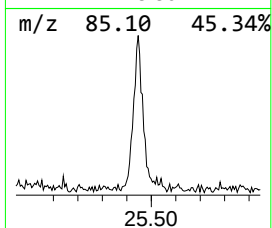
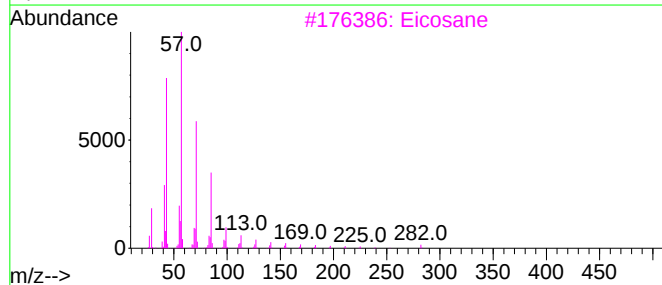
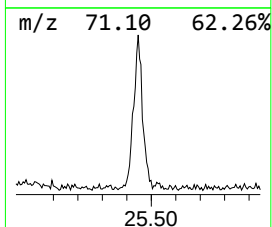
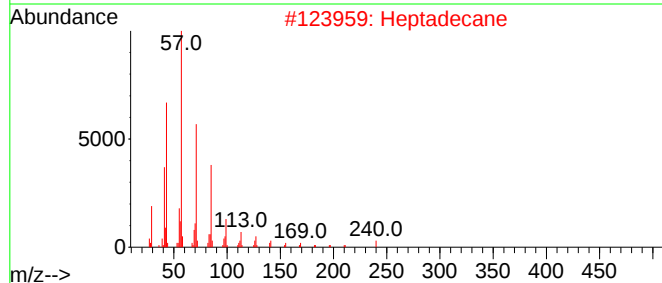
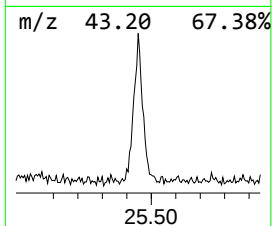
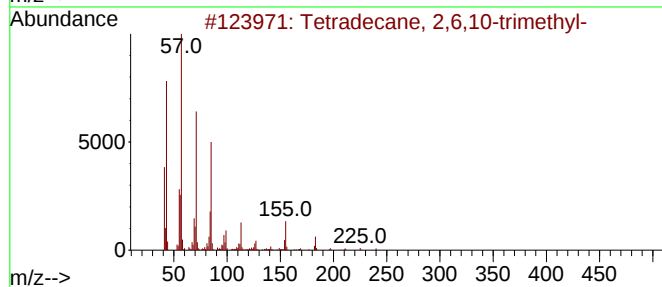
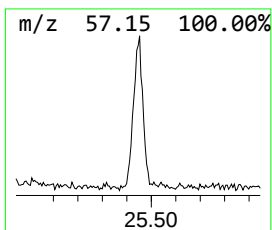
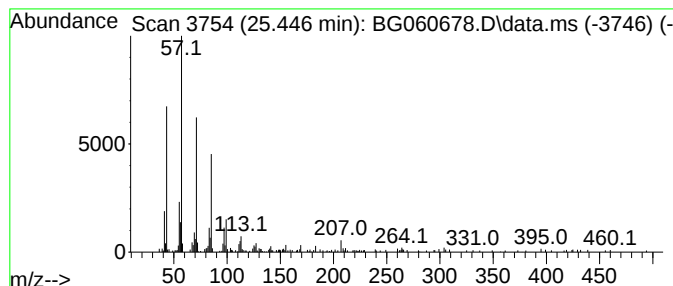
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tetradecane, 2,6,10-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.446	2.38 ng	255753	Perylene-d12	25.517

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	90
2		Heptadecane	240	C17H36	000629-78-7	80
3		Eicosane	282	C20H42	000112-95-8	80
4		Heptacosane	380	C27H56	000593-49-7	80
5		Pentadecane	212	C15H32	000629-62-9	72



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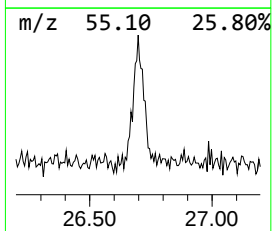
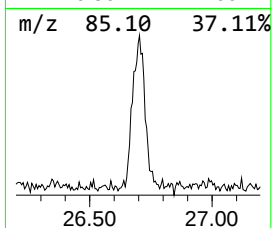
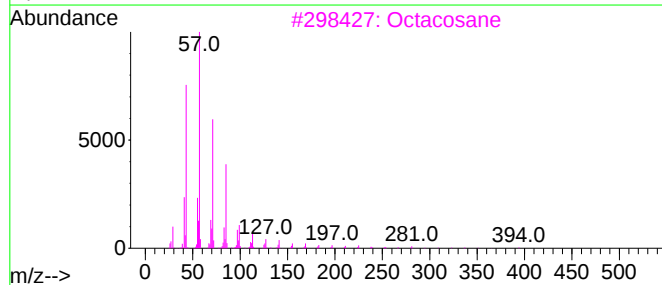
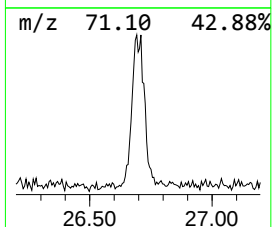
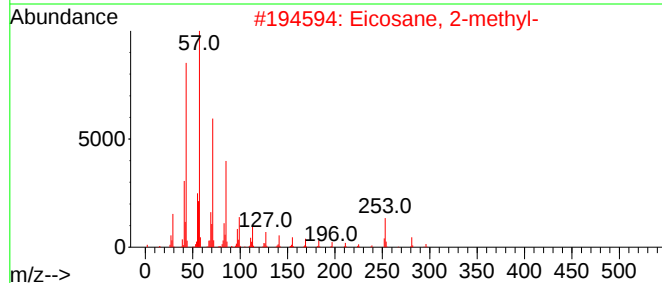
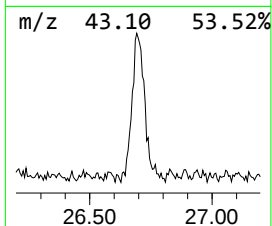
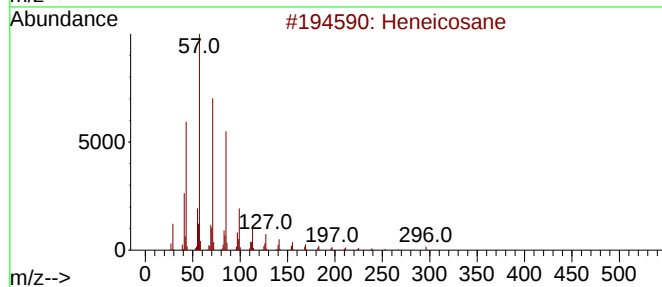
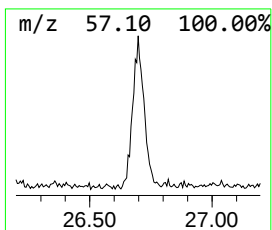
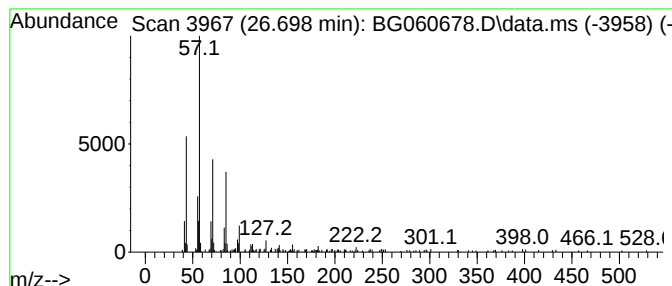
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.698	2.74 ng	294425	Perylene-d12	25.517

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	94
2			Eicosane, 2-methyl-	296	C21H44	001560-84-5	91
3			Octacosane	394	C28H58	000630-02-4	83
4			Undecane, 2-methyl-	170	C12H26	007045-71-8	80
5			Tetracosane	338	C24H50	000646-31-1	80



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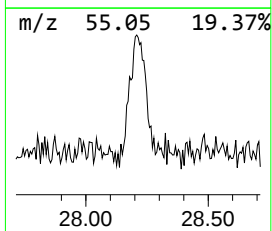
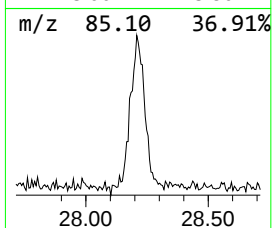
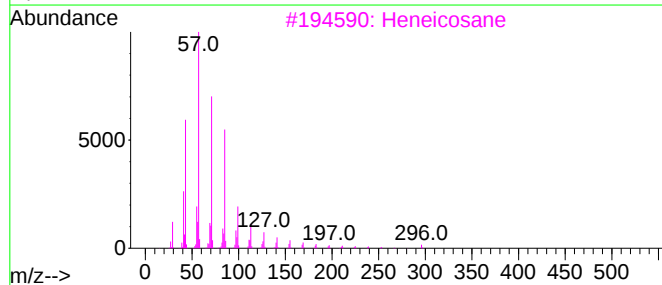
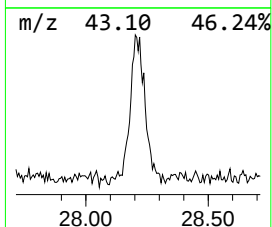
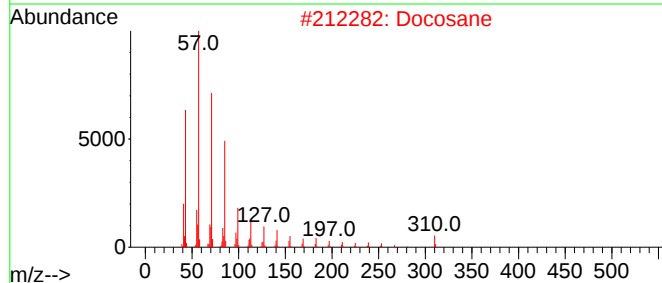
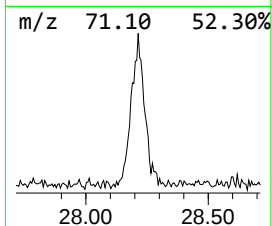
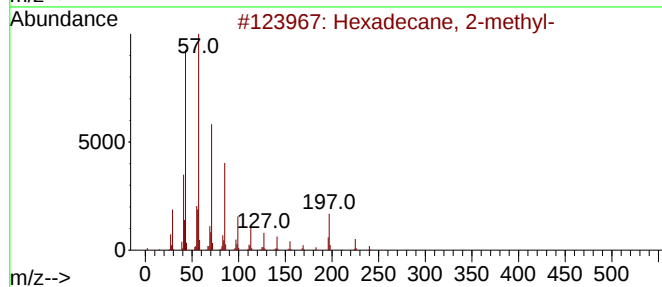
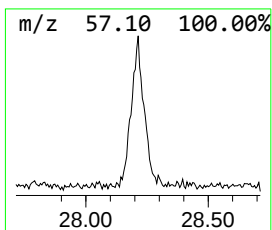
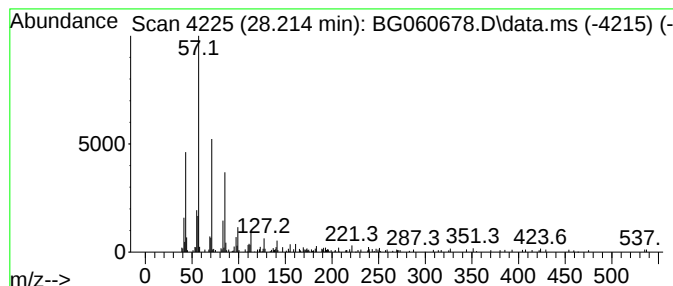
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Peak Number 5 Hexadecane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.214	2.87 ng	308817	Perylene-d12	25.517

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	74
2			Docosane	310	C22H46	000629-97-0	72
3			Heneicosane	296	C21H44	000629-94-7	72
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	72
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.323	5.5	ng	156428	1	8.290	567183	20.0
Hexadecanoic ac...	19.900	2.2	ng	212239	5	21.985	1917680	20.0
Tetradecane, 2,...	25.446	2.4	ng	255753	6	25.517	2148860	20.0
Heneicosane	26.698	2.7	ng	294425	6	25.517	2148860	20.0
Hexadecane, 2-m...	28.214	2.9	ng	308817	6	25.517	2148860	20.0