

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031919\
 Data File : BF113160.D
 Acq On : 20 Mar 2019 8:16
 Operator : JU/SJ
 Sample : K1948-04
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PST-026-B020-031319

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF022719.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.346	549	554	557	rBV	3665618	3960838	86.65%	11.381%
2	6.375	723	729	732	rBV	3787987	4570816	100.00%	13.133%
3	6.498	745	750	753	rBV	4088542	4132474	90.41%	11.874%
4	6.557	757	760	773	rVB	66677	96496	2.11%	0.277%
5	6.722	784	788	791	rBV	1222854	997077	21.81%	2.865%
6	6.881	810	815	818	rBV	3651971	3308863	72.39%	9.507%
7	7.287	878	884	887	rBV	2744084	2698032	59.03%	7.752%
8	8.004	1001	1006	1023	rBV	1315032	1286143	28.14%	3.695%
9	9.081	1183	1189	1192	rBV	4321614	3946269	86.34%	11.339%
10	9.469	1252	1255	1264	rBV	289860	285303	6.24%	0.820%
11	9.751	1297	1303	1315	rVB2	1150111	1092000	23.89%	3.138%
12	10.539	1433	1437	1448	rBV	2156915	2151615	47.07%	6.182%
13	11.233	1551	1555	1562	rBV	989407	921083	20.15%	2.647%
14	11.769	1643	1646	1657	rBV2	194498	226247	4.95%	0.650%
15	12.551	1776	1779	1789	rBV2	42554	63802	1.40%	0.183%
16	12.816	1819	1824	1827	rBV	3119933	2820447	61.71%	8.104%
17	13.733	1975	1980	1995	rBV4	112585	308826	6.76%	0.887%
18	13.863	1997	2002	2009	rVB	817541	844178	18.47%	2.426%
19	14.339	2080	2083	2086	rBV	52086	46048	1.01%	0.132%
20	14.374	2086	2089	2100	rVB7	26806	64583	1.41%	0.186%
21	14.633	2130	2133	2137	rVB	64082	58885	1.29%	0.169%
22	14.951	2183	2187	2191	rBV	88897	89660	1.96%	0.258%
23	15.021	2193	2199	2205	rBV8	23215	53079	1.16%	0.153%
24	15.268	2236	2241	2245	rBV	476769	609671	13.34%	1.752%
25	15.304	2245	2247	2253	rVB	67835	80842	1.77%	0.232%
26	15.704	2311	2315	2320	rVB	66227	90266	1.97%	0.259%

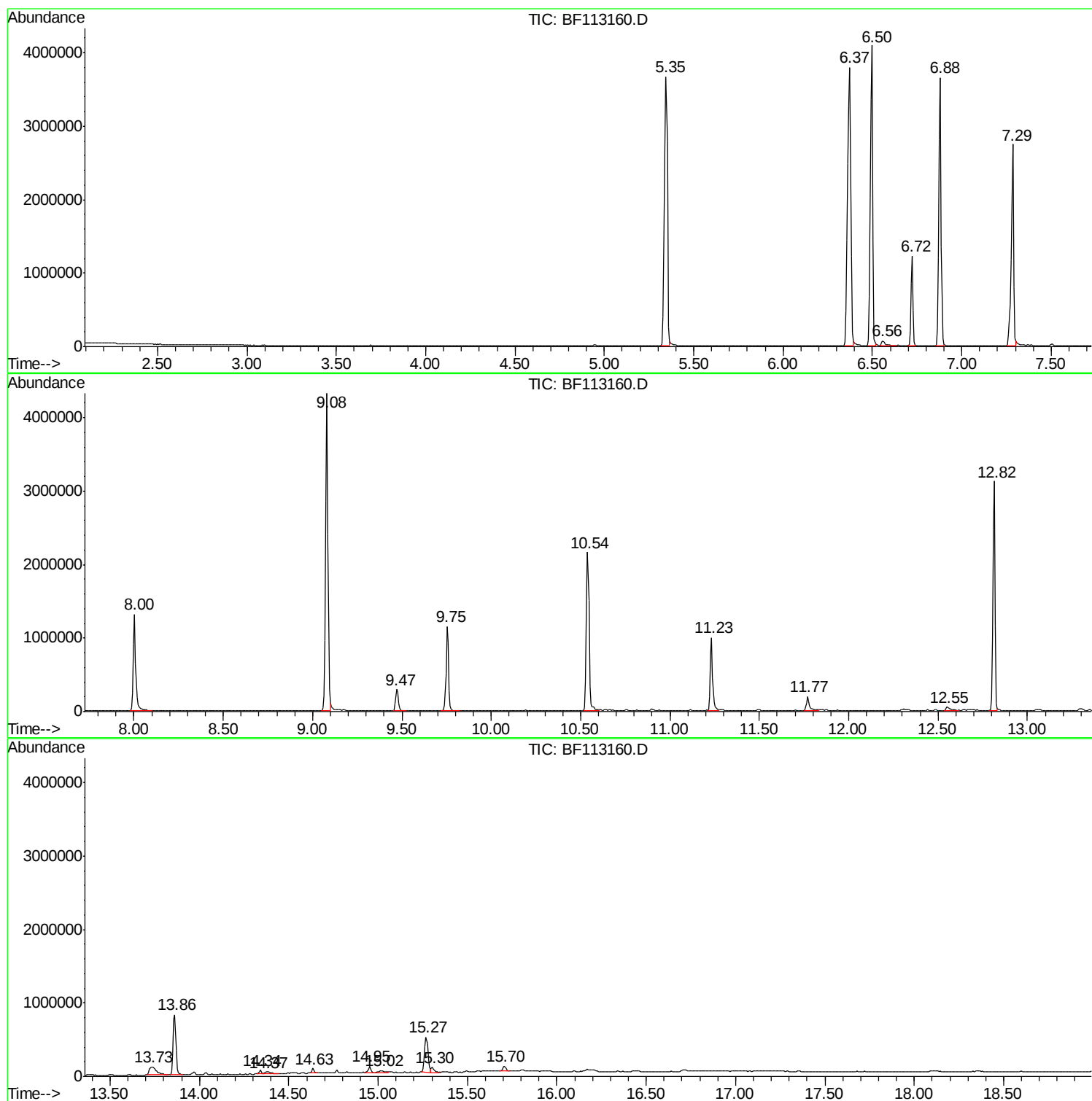
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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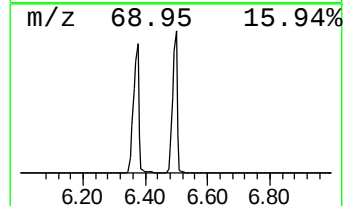
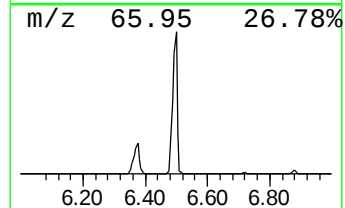
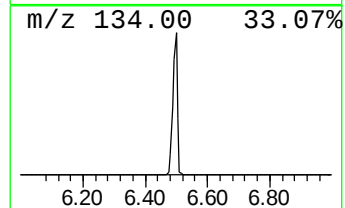
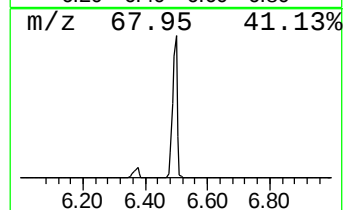
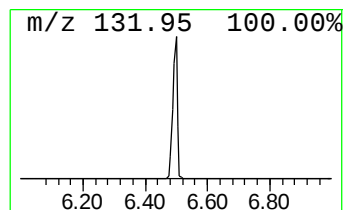
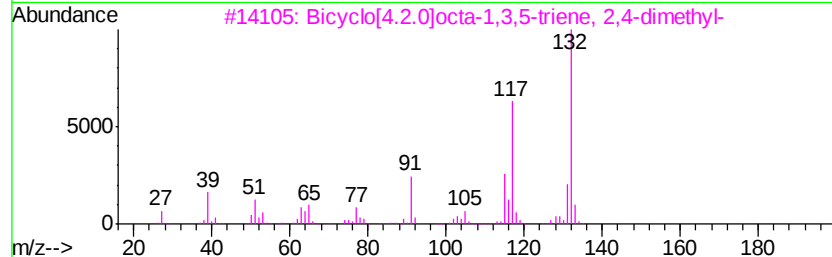
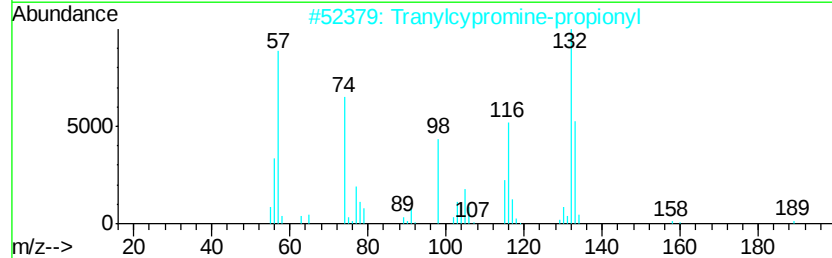
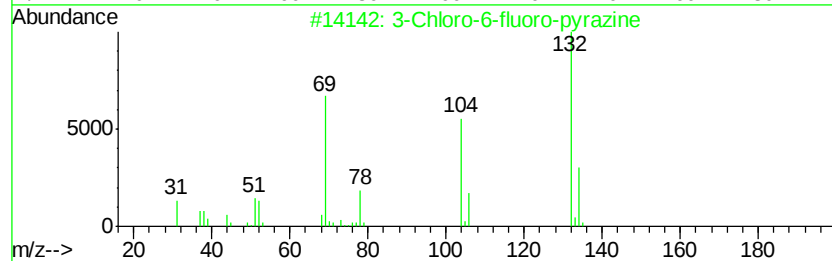
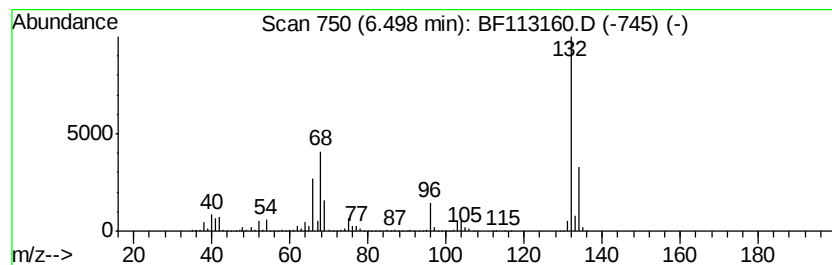
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	82.89 ng	4132470	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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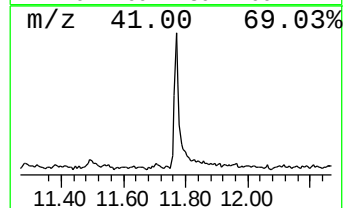
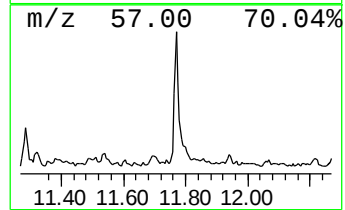
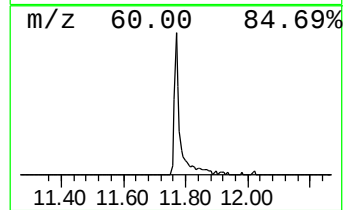
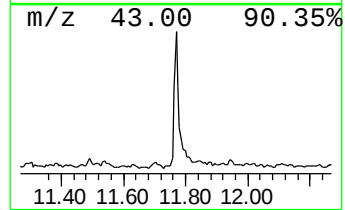
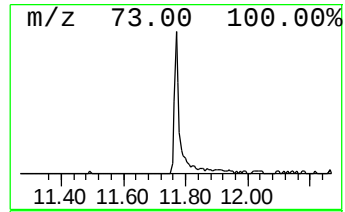
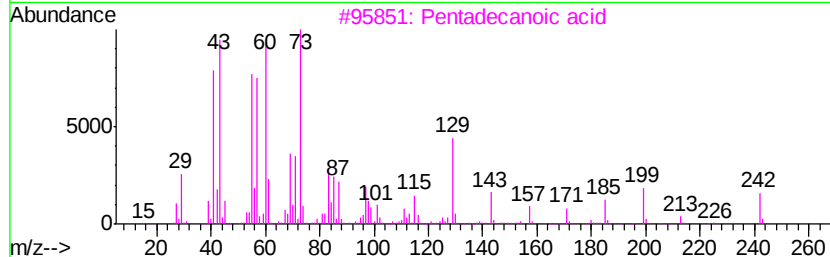
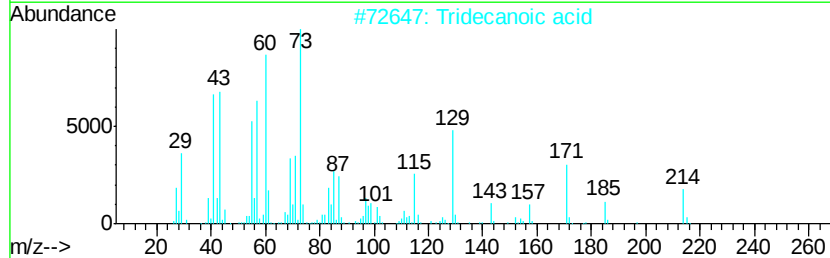
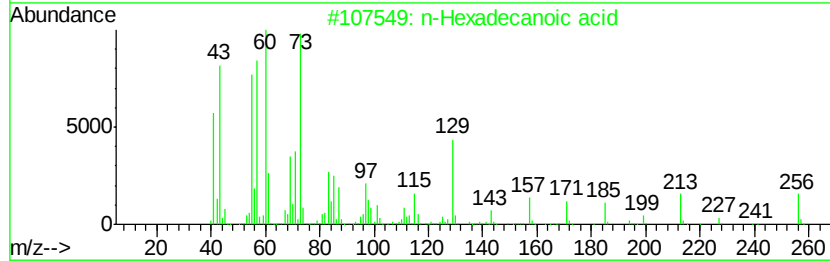
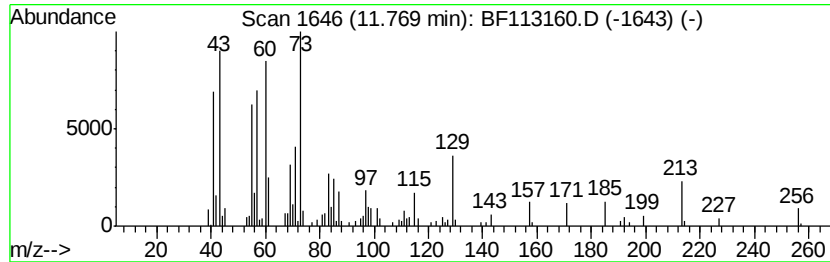
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	4.91 ng	226247	Phenanthrene-d10	11.23	
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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	18



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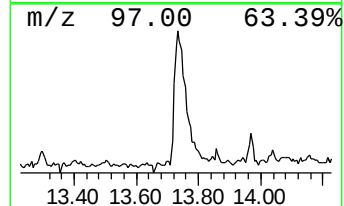
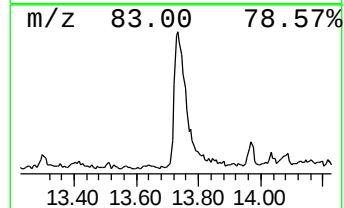
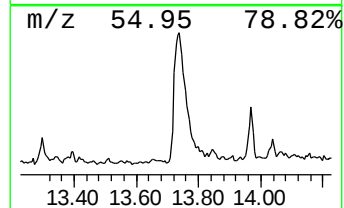
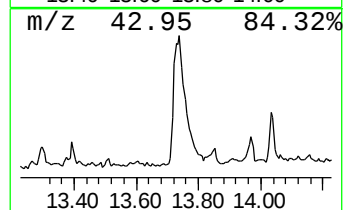
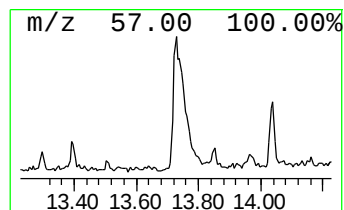
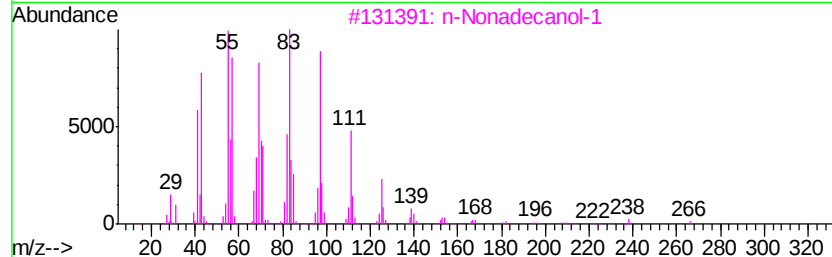
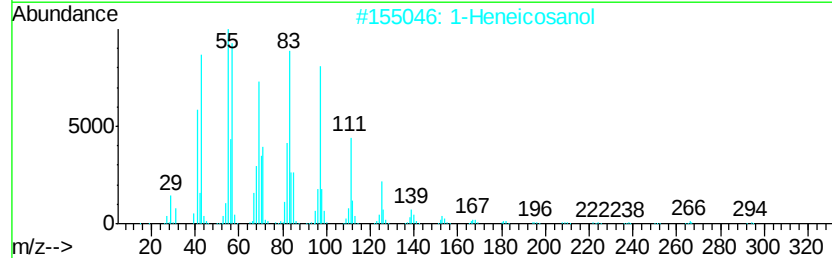
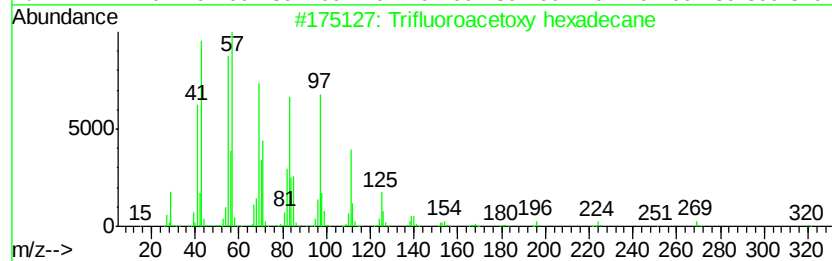
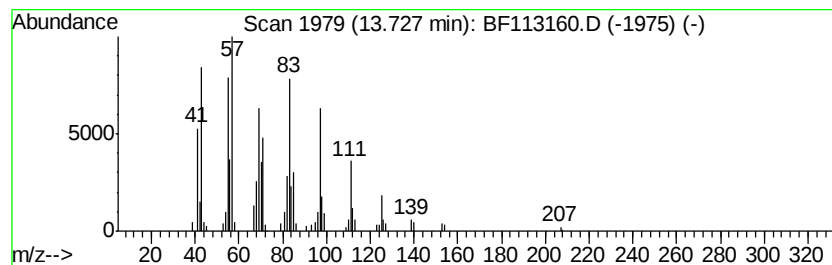
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Trifluoroacetoxy hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.73	7.32 ng	308826	Chrysene-d12		13.86		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			Behenic alcohol	326	C22H46O	000661-19-8	93



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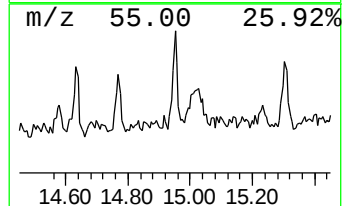
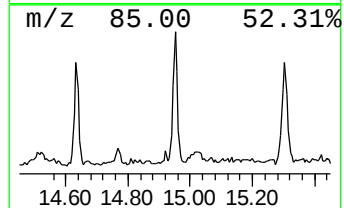
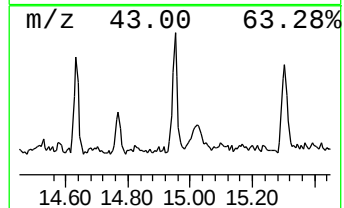
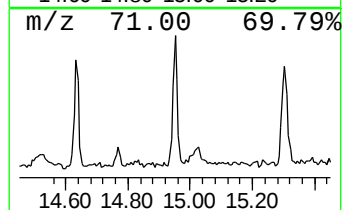
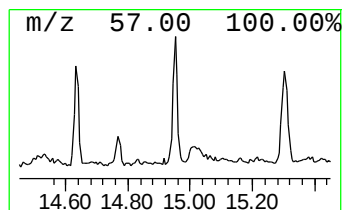
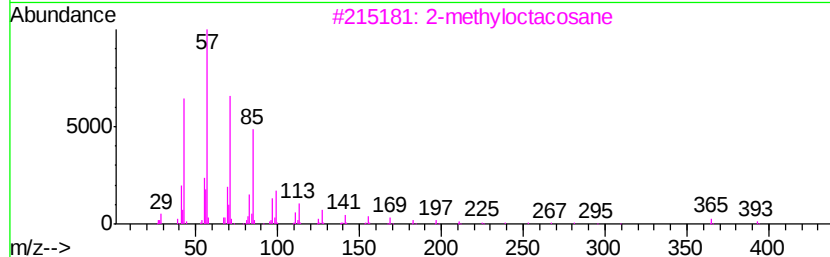
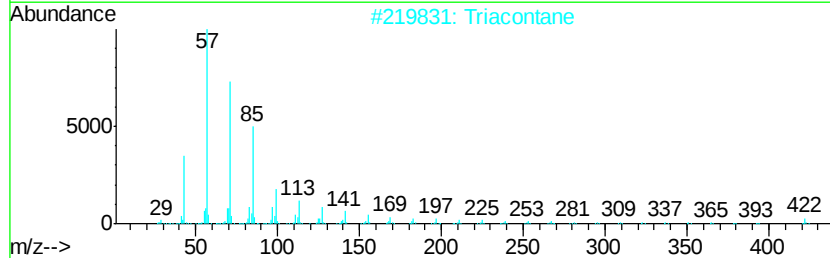
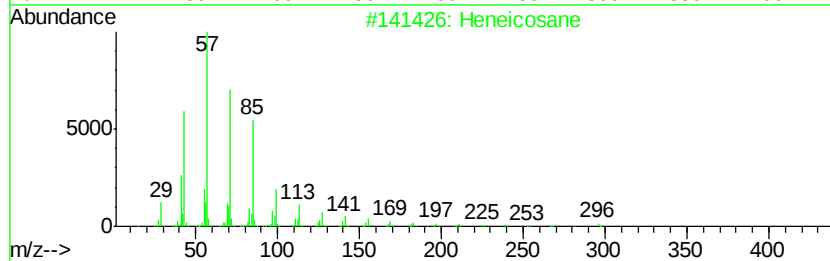
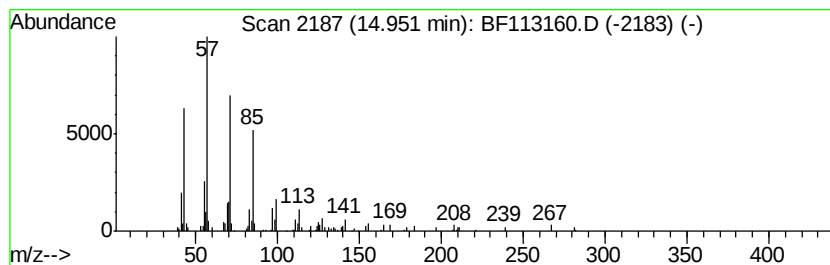
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Peak Number 4 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.94 ng	89660	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Triacontane		422	C30H62	000638-68-6	91
3	2-methyloctacosane		408	C29H60	1000376-72-8	91
4	Octacosane		394	C28H58	000630-02-4	91
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91



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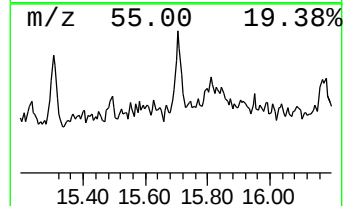
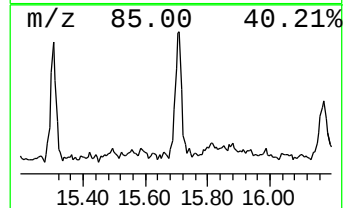
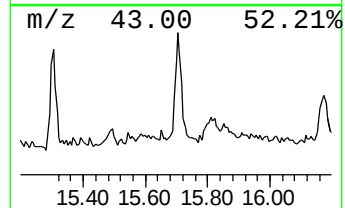
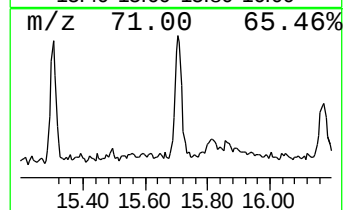
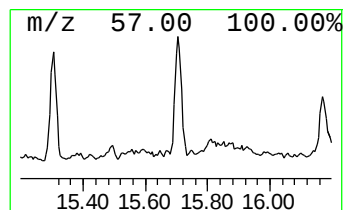
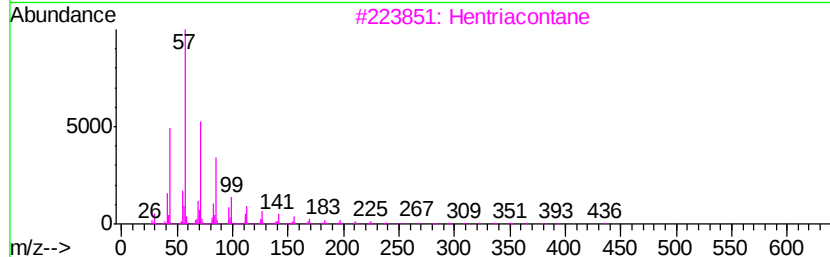
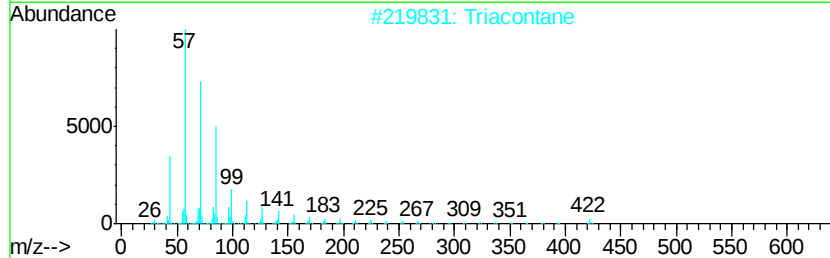
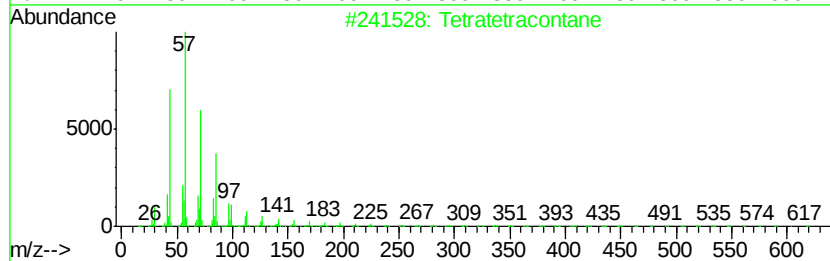
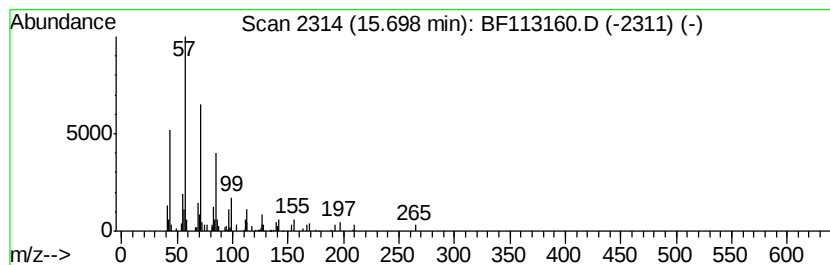
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetratetracontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	2.96 ng	90266	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	91
2		triacontane	422	C30H62	000638-68-6	91
3		hentriacontane	437	C31H64	000630-04-6	91
4		heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		docosane, 11-decyl-	451	C32H66	055401-55-3	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.50	6.50	82.9	ng	4132470	1	6.72	997077	20.0
n-Hexadecanoic acid	11.77	4.9	ng	226247	4	11.23	921083	20.0
Trifluoroacetoxy ...	13.73	7.3	ng	308826	5	13.86	844178	20.0
Heneicosane	14.95	2.9	ng	89660	6	15.27	609671	20.0
Tetratetracontane	15.70	3.0	ng	90266	6	15.27	609671	20.0