

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109666.D
Acq On : 8 Oct 2018 23:49
Operator : JU/SJ
Sample : J5294-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HP-SUB

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-BF100818.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	4.922	479	482	497	rBV	62710	116993	3.61%	0.456%
2	5.328	547	551	583	rBV	2180564	2915517	90.02%	11.357%
3	6.357	721	726	741	rBV	2176388	3102779	95.80%	12.087%
4	6.475	741	746	770	rVB	2769765	3238911	100.00%	12.617%
5	6.698	781	784	806	rVB	479538	658662	20.34%	2.566%
6	6.851	806	810	840	rVB	2161936	2426107	74.91%	9.451%
7	7.263	875	880	908	rBV	1614698	2058936	63.57%	8.021%
8	7.975	998	1001	1024	rBV	584783	798192	24.64%	3.109%
9	9.051	1179	1184	1207	rBV	3003073	3212920	99.20%	12.516%
10	9.445	1247	1251	1262	rBV	118995	133820	4.13%	0.521%
11	9.722	1294	1298	1316	rBV	793188	788700	24.35%	3.072%
12	10.510	1428	1432	1449	rBV	1454651	1727937	53.35%	6.731%
13	11.204	1546	1550	1560	rBV	554844	685560	21.17%	2.671%
14	12.633	1784	1793	1796	rBV2	29308	36411	1.12%	0.142%
15	12.780	1814	1818	1828	rBV	2235847	2139754	66.06%	8.335%
16	13.686	1968	1972	1987	rBV3	101841	177152	5.47%	0.690%
17	13.827	1991	1996	2008	rVV	573453	644673	19.90%	2.511%
18	14.298	2073	2076	2081	rBV	37560	37085	1.14%	0.144%
19	14.592	2123	2126	2133	rBV	50393	47040	1.45%	0.183%
20	14.904	2175	2179	2182	rBV	50258	48711	1.50%	0.190%
21	15.221	2229	2233	2237	rBV	397214	515403	15.91%	2.008%
22	15.645	2300	2305	2310	rBV2	46999	65141	2.01%	0.254%
23	16.104	2378	2383	2387	rBV3	35051	59948	1.85%	0.234%
24	16.633	2469	2473	2480	rVB3	17641	34222	1.06%	0.133%

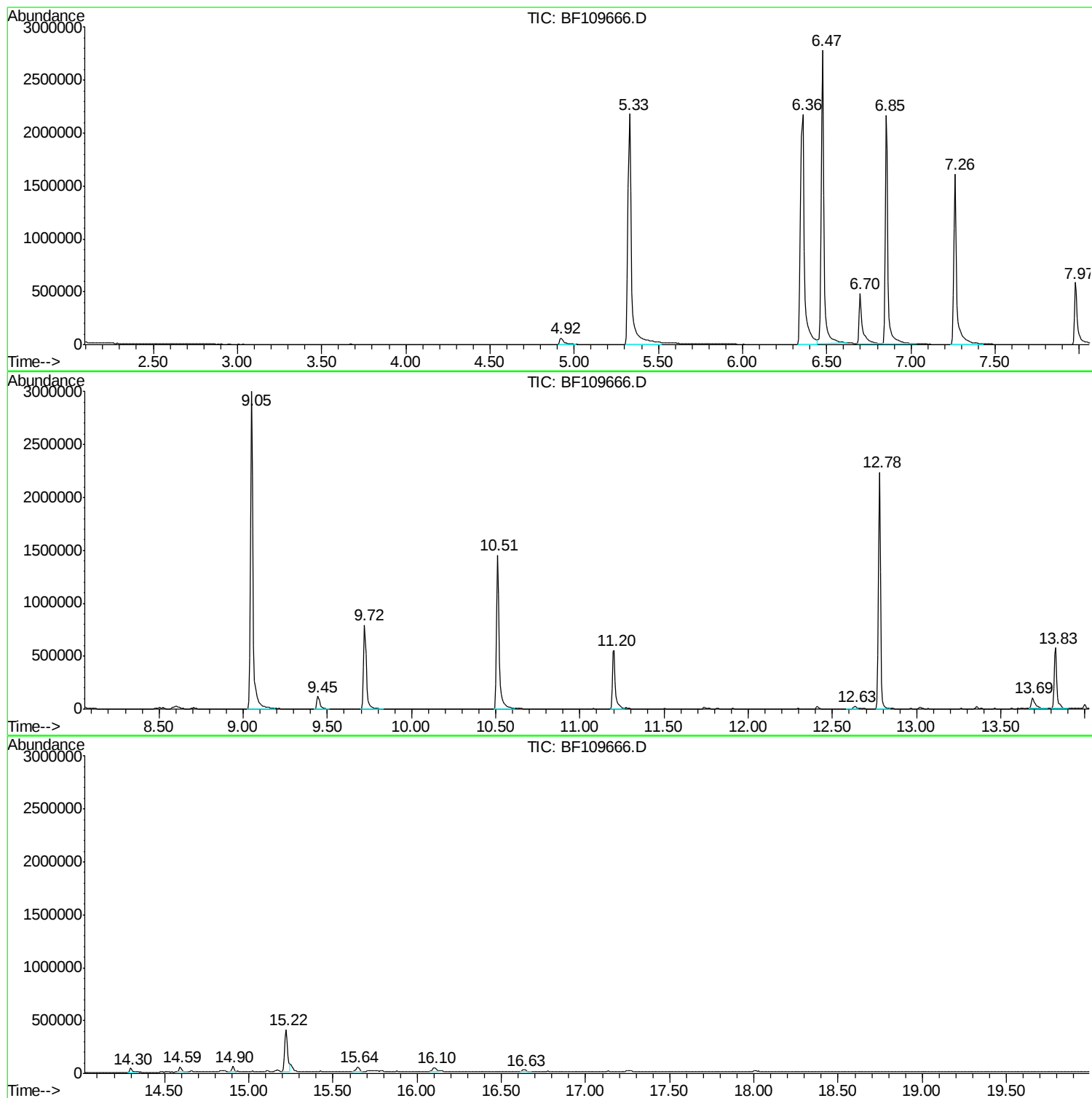
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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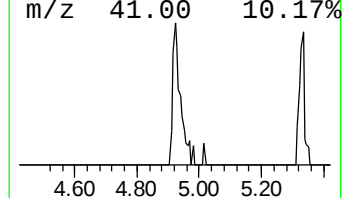
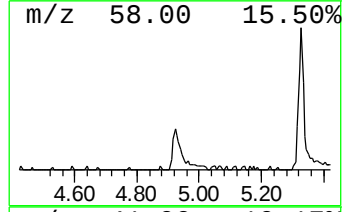
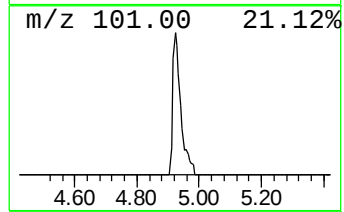
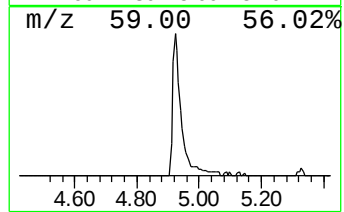
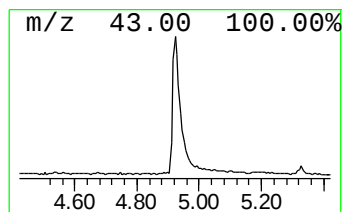
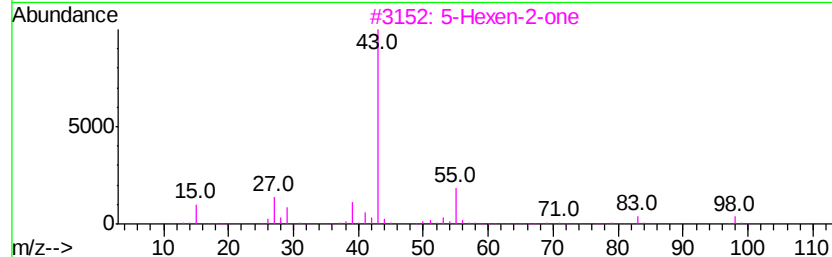
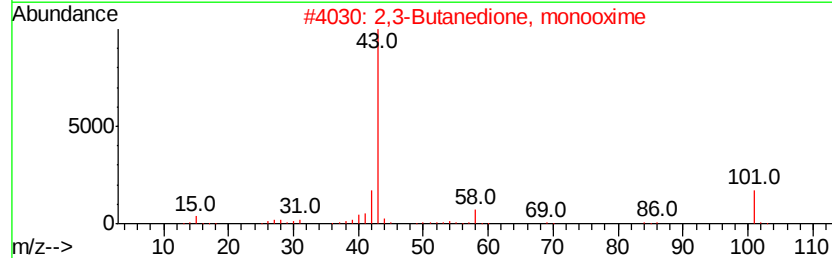
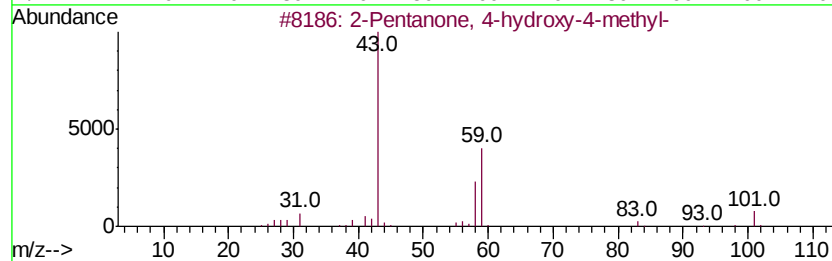
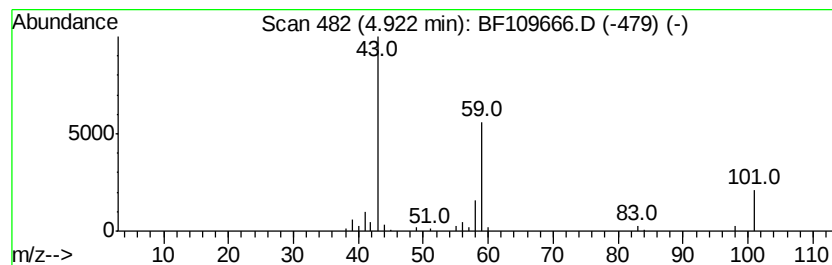
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	3.55 ng	116993	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Propylamine	59	C3H9N	000107-10-8	9
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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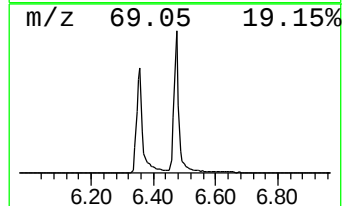
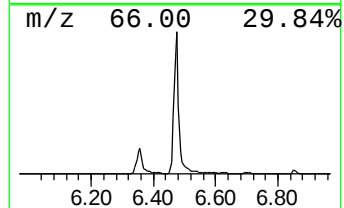
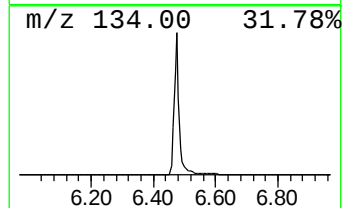
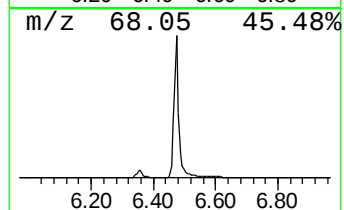
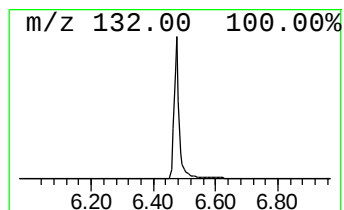
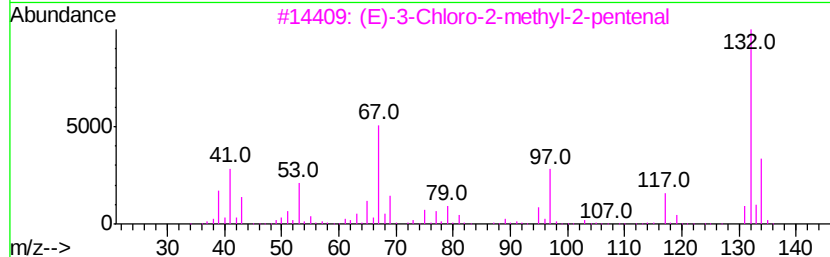
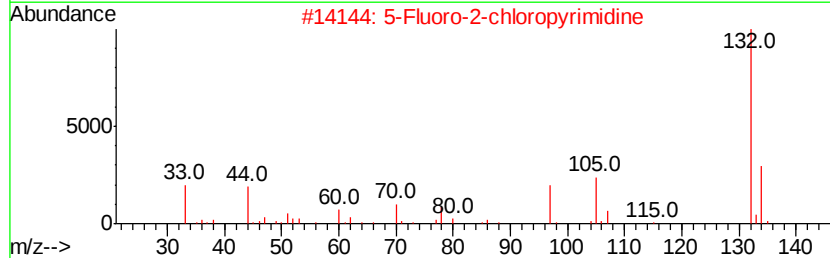
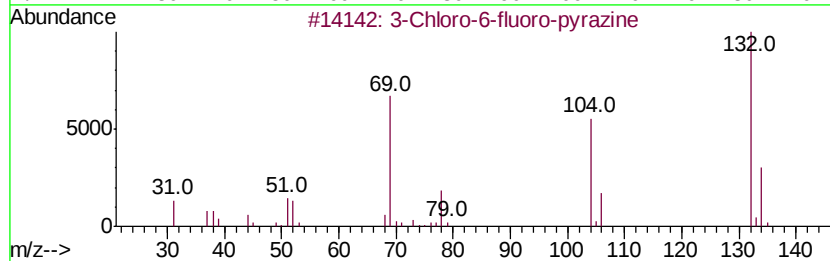
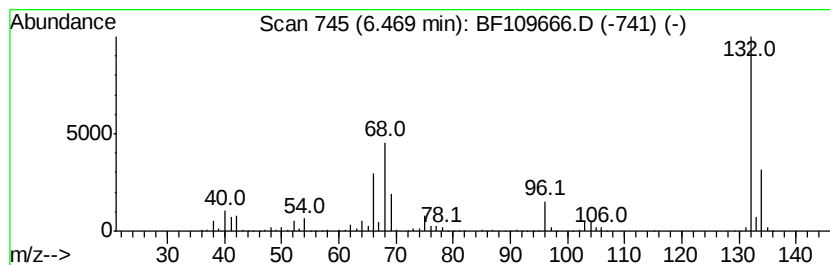
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	98.35 ng	3238910	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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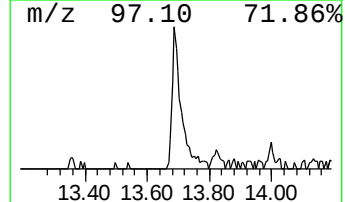
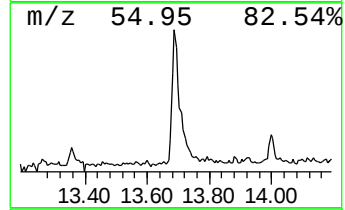
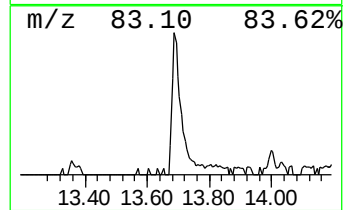
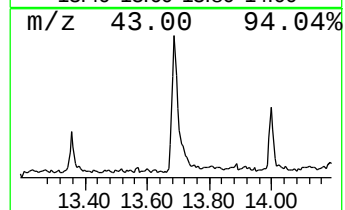
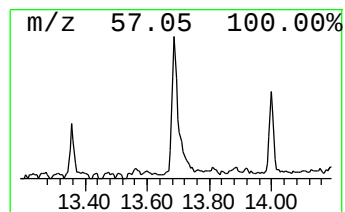
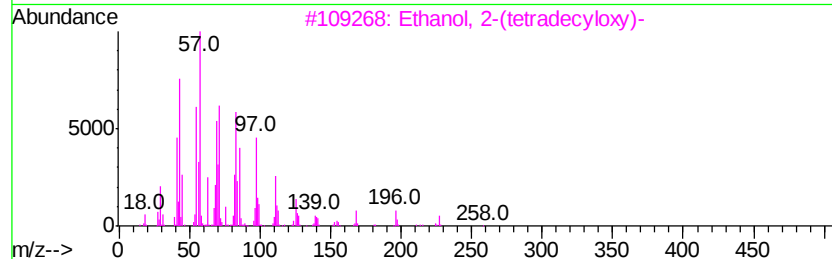
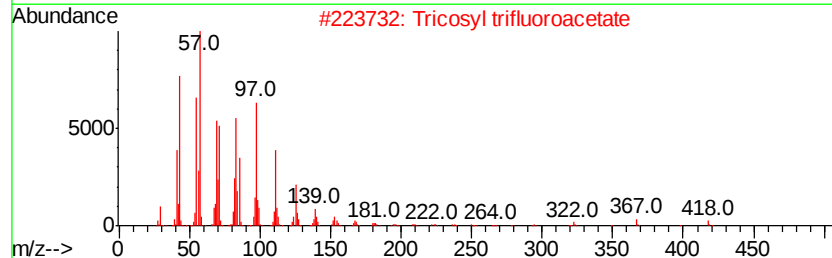
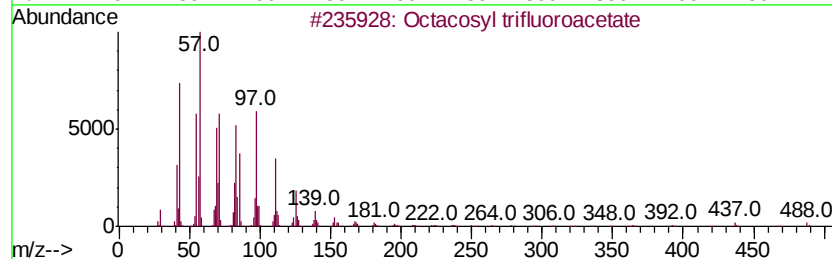
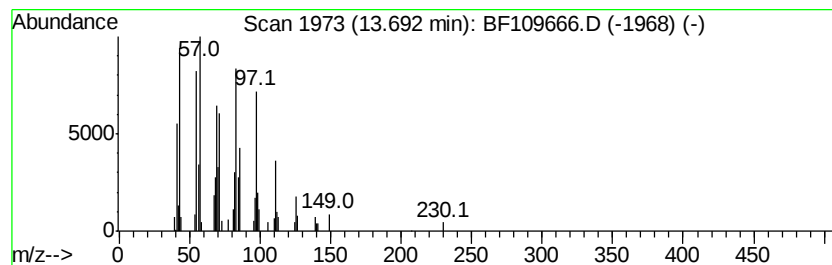
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Peak Number 4 Octacosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	5.50 ng	177152	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
2		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
3		Ethanol, 2-(tetradecyl)-	258	C16H34O2	002136-70-1	90
4		Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	87
5		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87



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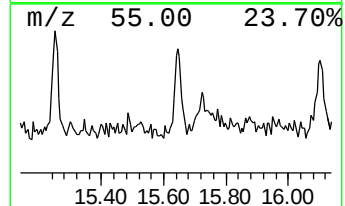
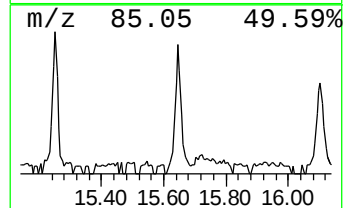
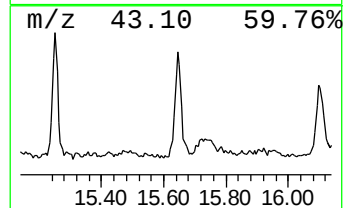
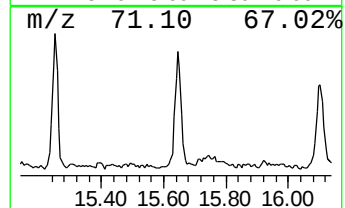
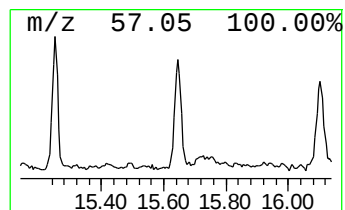
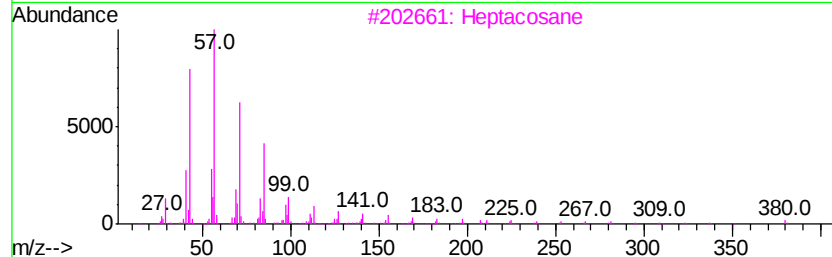
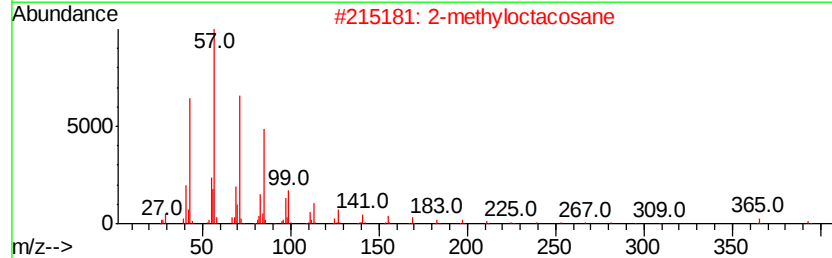
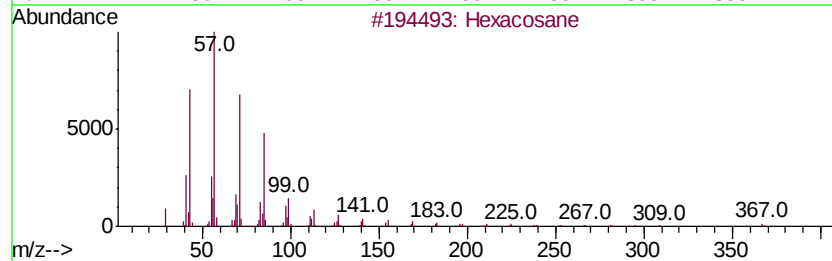
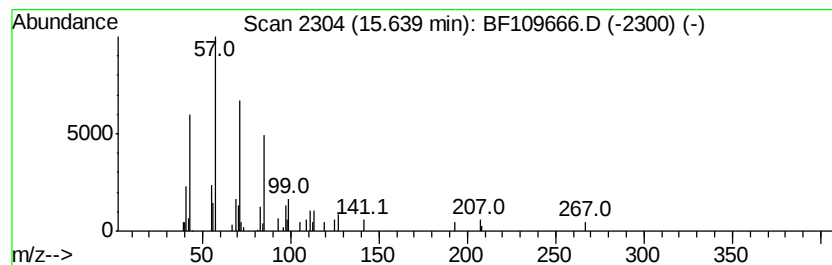
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Peak Number 5 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	2.53 ng	65141	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Heneicosane	296	C21H44	000629-94-7	87
5		Octacosane	394	C28H58	000630-02-4	87



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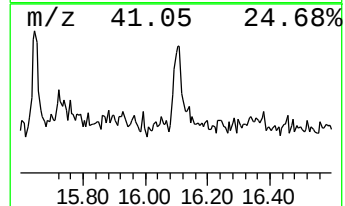
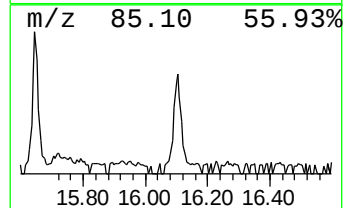
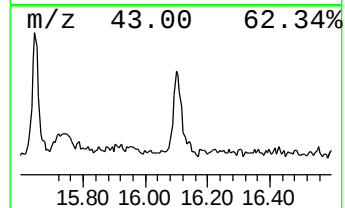
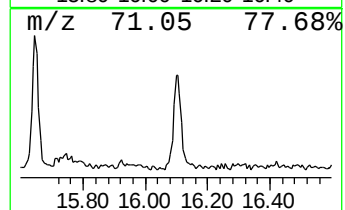
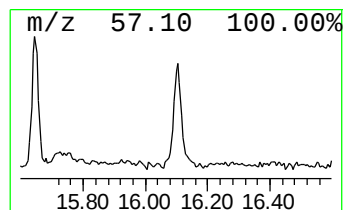
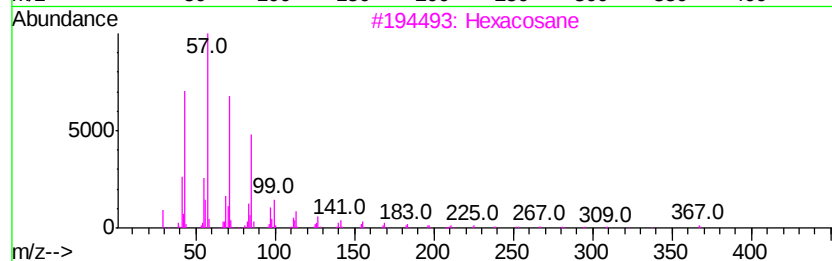
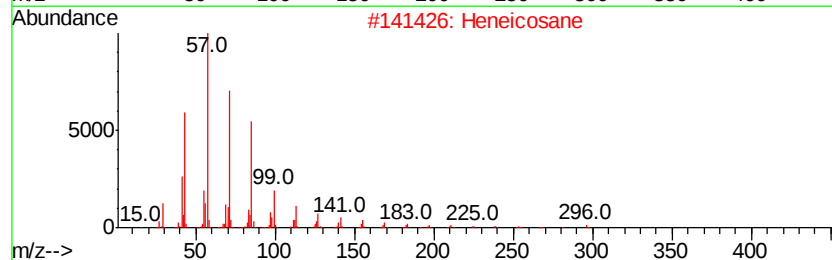
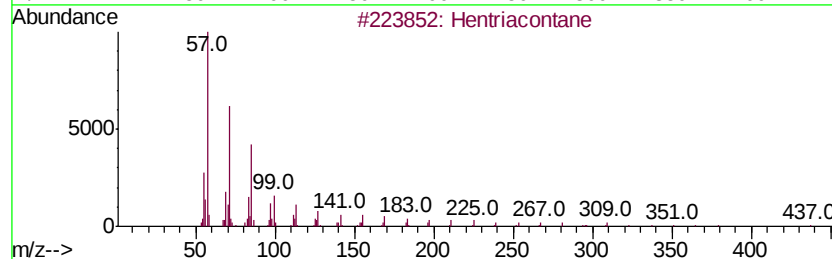
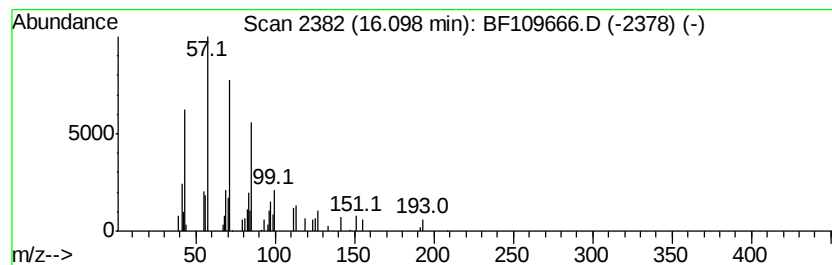
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.33 ng	59948	Perylene-d12	15.22

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	90
2	Heneicosane		296	C21H44	000629-94-7	87
3	Hexacosane		366	C26H54	000630-01-3	87
4	Octacosane		394	C28H58	000630-02-4	87
5	Hexatriacontane		507	C36H74	000630-06-8	86



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	3.5	ng	116993	1	6.70	658662	20.0
unknown6.47	6.47	98.3	ng	3238910	1	6.70	658662	20.0
Octacosyl trifluo...	13.69	5.5	ng	177152	5	13.83	644673	20.0
Hexacosane	15.64	2.5	ng	65141	6	15.22	515403	20.0
Hentriacontane	16.10	2.3	ng	59948	6	15.22	515403	20.0