

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100918\
 Data File : BF109693.D
 Acq On : 9 Oct 2018 14:22
 Operator : JU/SJ
 Sample : PB113605BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB113605BL

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-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	492	rBV	49760	72953	2.42%	0.304%
2	5.328	547	551	580	rBV	1579735	2016131	66.76%	8.410%
3	6.345	720	724	741	rBV	1532731	2200671	72.87%	9.179%
4	6.469	741	745	770	rVB	2024893	2376467	78.69%	9.913%
5	6.698	780	784	806	rVV	390289	596548	19.75%	2.488%
6	6.851	806	810	848	rVB	1653035	1851589	61.31%	7.723%
7	7.257	875	879	923	rBV	945941	1539775	50.99%	6.423%
8	7.975	997	1001	1031	rBV	546332	810510	26.84%	3.381%
9	9.051	1178	1184	1219	rBV	2543478	2990404	99.02%	12.473%
10	9.722	1292	1298	1318	rBV2	858421	960882	31.82%	4.008%
11	10.510	1428	1432	1459	rBV	1443573	1910187	63.25%	7.968%
12	11.204	1546	1550	1575	rBV	871087	1052452	34.85%	4.390%
13	12.786	1814	1819	1834	rBV	2884164	3019866	100.00%	12.596%
14	13.827	1992	1996	2009	rBV	899868	995846	32.98%	4.154%
15	14.304	2071	2077	2081	rBV2	30016	35717	1.18%	0.149%
16	14.598	2120	2127	2131	rBV	75475	82162	2.72%	0.343%
17	14.910	2173	2180	2189	rBV	111593	136500	4.52%	0.569%
18	15.227	2229	2234	2249	rBV	616261	1048391	34.72%	4.373%
19	15.651	2299	2306	2312	rBV	111867	155964	5.16%	0.651%
20	16.109	2376	2384	2390	rBV	49924	89597	2.97%	0.374%
21	16.645	2469	2475	2480	rVB2	16422	31600	1.05%	0.132%

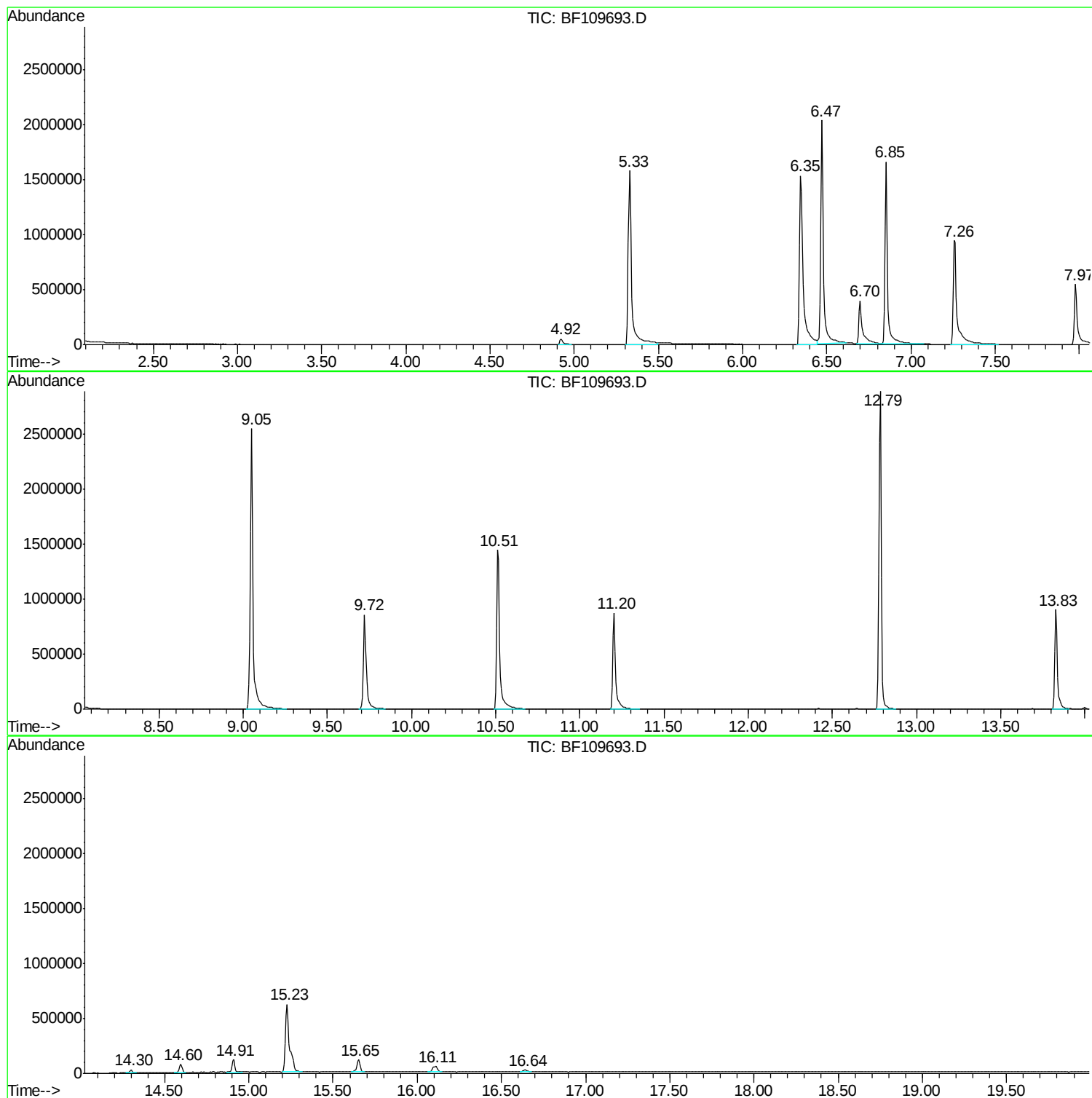
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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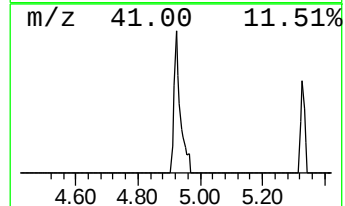
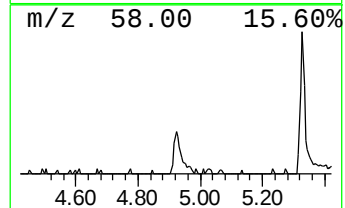
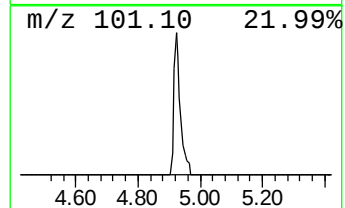
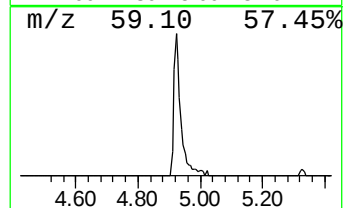
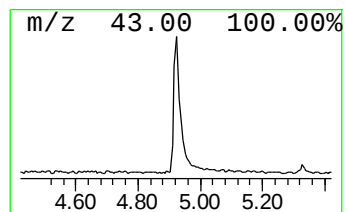
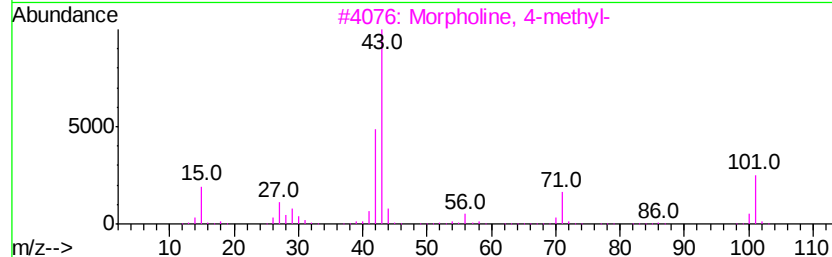
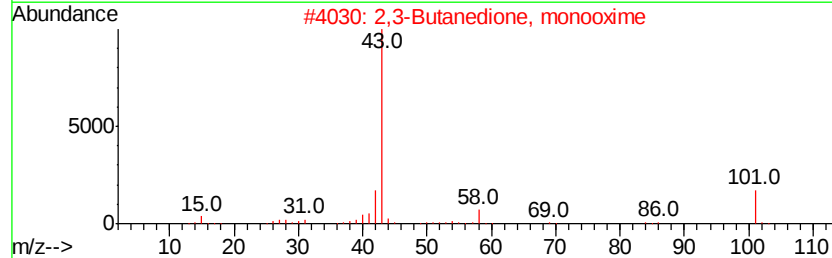
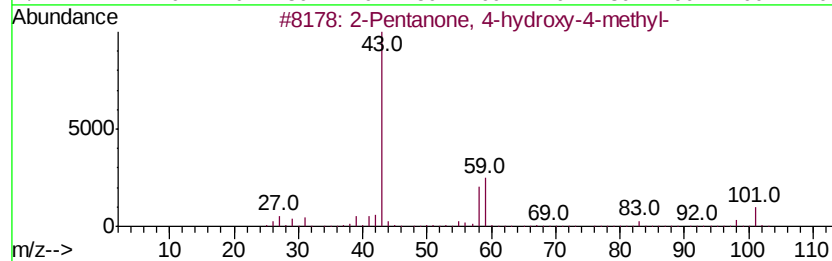
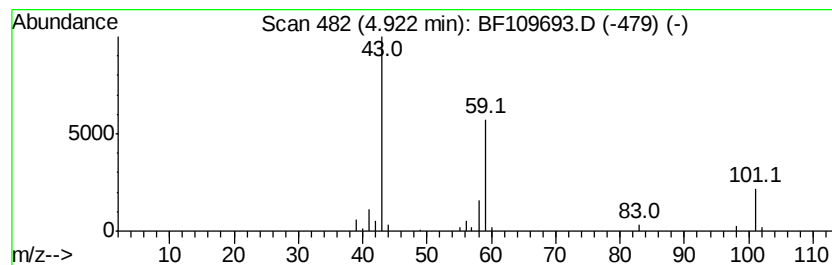
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	2.45 ng	72953	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	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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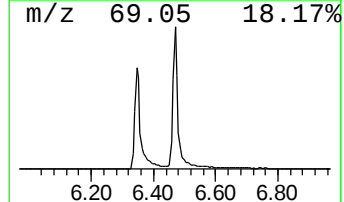
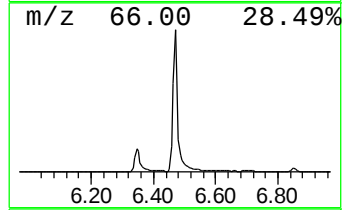
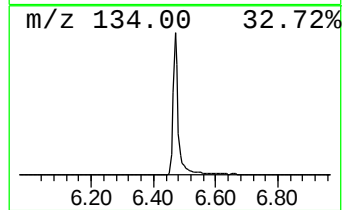
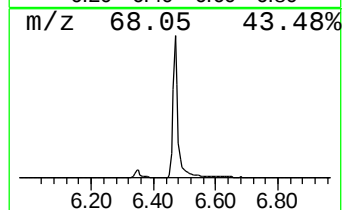
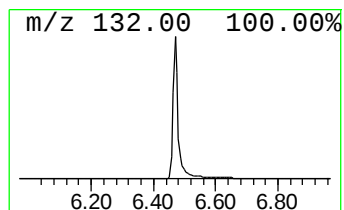
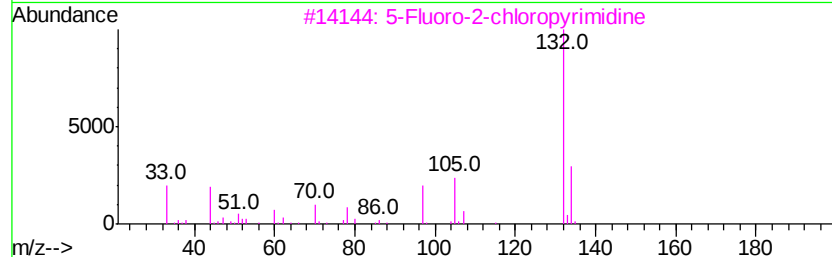
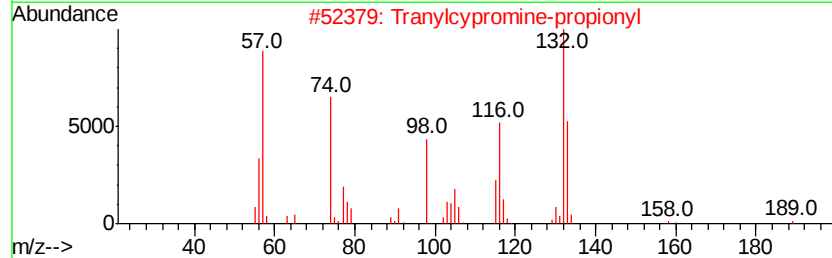
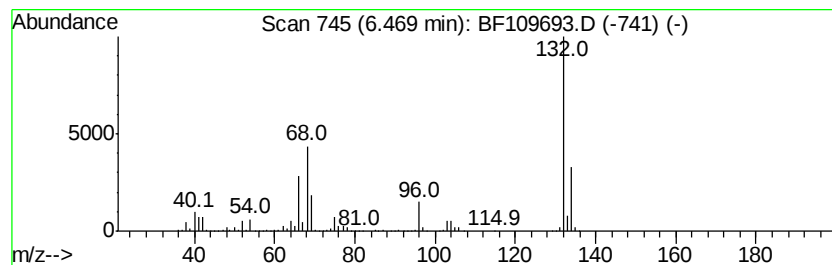
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	79.67 ng	2376470	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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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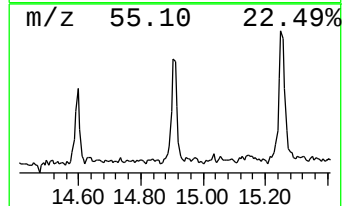
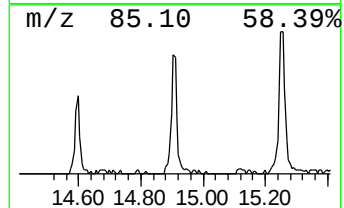
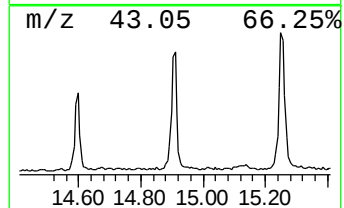
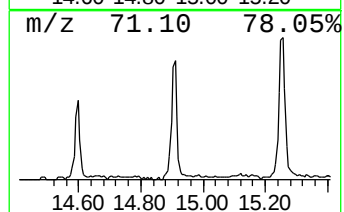
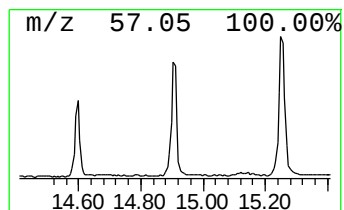
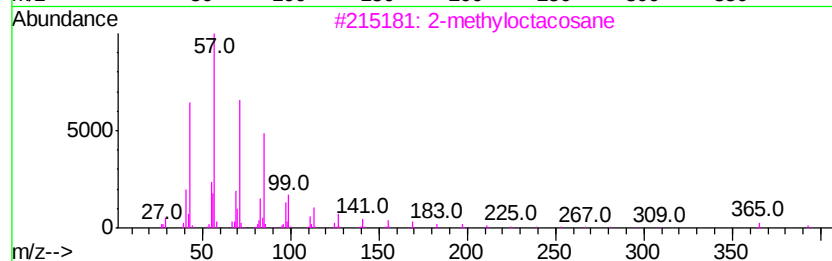
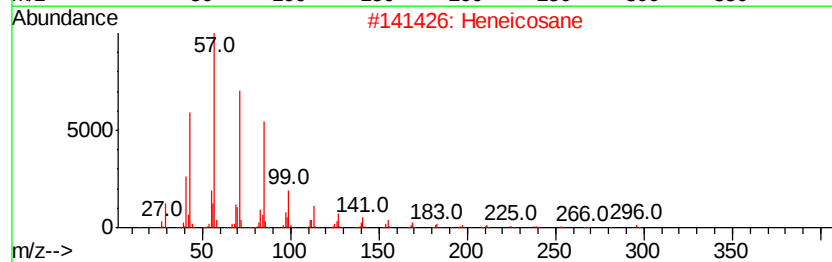
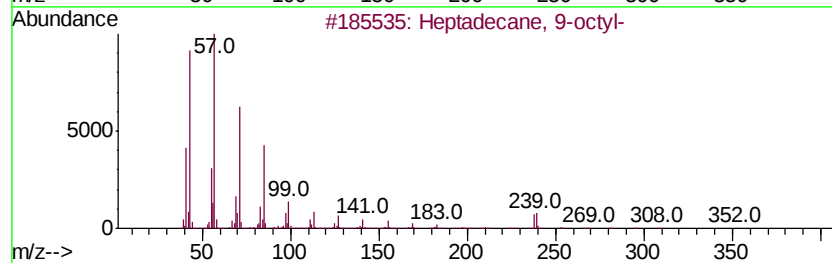
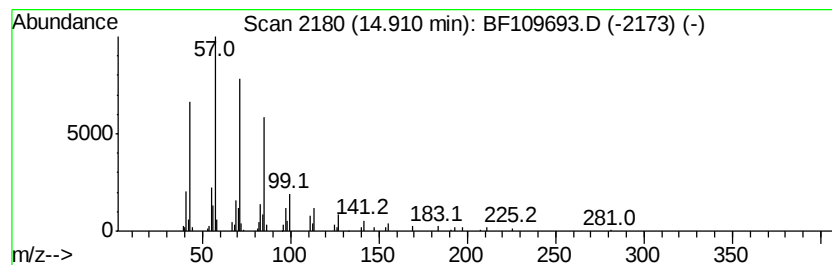
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Peak Number 4 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	2.60 ng	136500	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Octacosane	394	C28H58	000630-02-4	91



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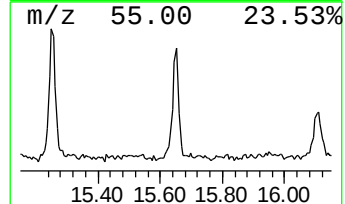
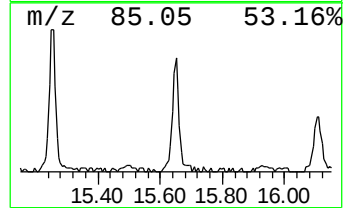
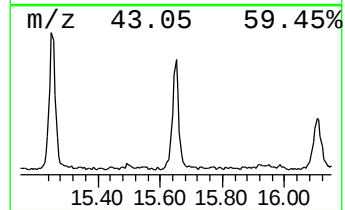
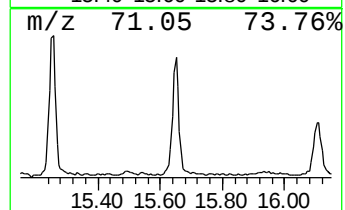
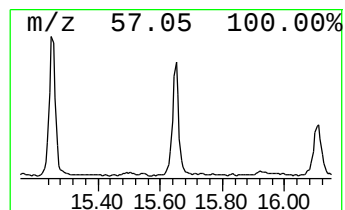
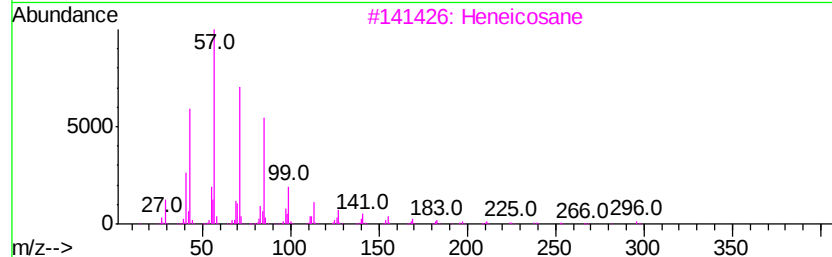
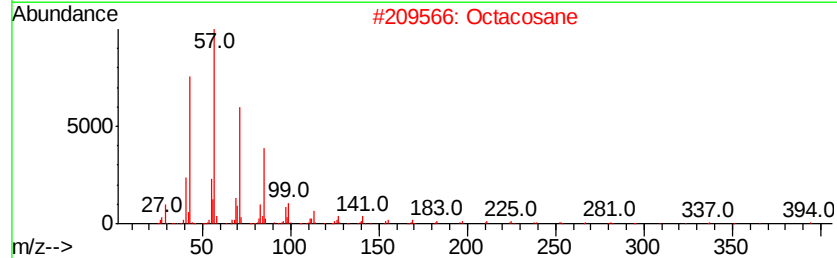
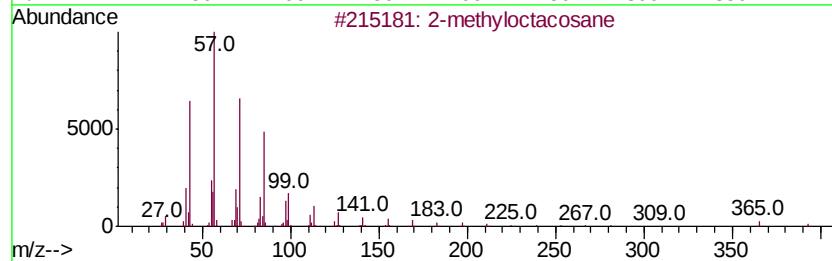
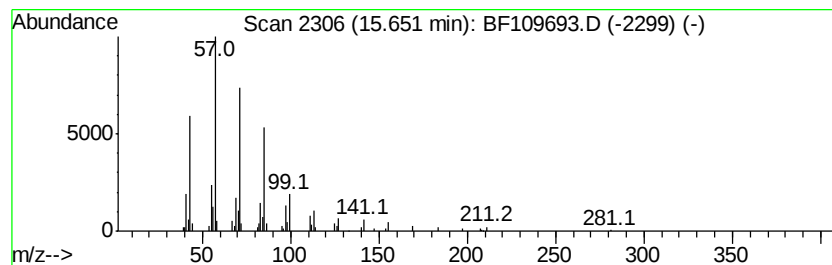
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Peak Number 5 2-methyloctacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	2.98 ng	155964	Perylene-d12	15.23

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



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	2.5	ng	72953	1	6.70	596548	20.0
unknown6.47	6.47	79.7	ng	2376470	1	6.70	596548	20.0
Heptadecane, 9-oc...	14.91	2.6	ng	136500	6	15.23	1048390	20.0
2-methyloctacosane	15.65	3.0	ng	155964	6	15.23	1048390	20.0