

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060117\
 Data File : BF095595.D
 Acq On : 1 Jun 2017 15:24
 Operator : SJ/MA
 Sample : PB99358BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB99358BL

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:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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	4.810	526	531	554	rBV	74051	210318	7.65%	0.956%
2	5.463	637	642	677	rBV	1215535	2394493	87.06%	10.881%
3	7.087	914	918	932	rBV	1347099	2241897	81.51%	10.187%
4	7.192	932	936	951	rVB	1739821	2629198	95.60%	11.947%
5	7.534	990	994	1009	rVB	373208	499067	18.15%	2.268%
6	7.775	1029	1035	1058	rBV	1390383	1933000	70.28%	8.784%
7	8.445	1144	1149	1176	rBV	832790	1291495	46.96%	5.869%
8	9.569	1335	1340	1360	rBV	430737	652377	23.72%	2.964%
9	11.345	1635	1642	1660	rBV	1966362	2727340	99.16%	12.393%
10	12.392	1814	1820	1831	rBV2	572341	791181	28.77%	3.595%
11	13.692	2036	2041	2066	rBV	966545	1394756	50.71%	6.338%
12	14.798	2224	2229	2241	rBV	547254	779374	28.34%	3.542%
13	16.880	2574	2583	2592	rBV5	12863	33003	1.20%	0.150%
14	17.151	2623	2629	2632	rBV	2221554	2750332	100.00%	12.498%
15	18.492	2853	2857	2872	rBV	592003	779900	28.36%	3.544%
16	20.168	3137	3142	3153	rBV	396537	602124	21.89%	2.736%
17	20.250	3153	3156	3161	rVB	43202	50307	1.83%	0.229%
18	20.609	3212	3217	3221	rVB	51606	65564	2.38%	0.298%
19	21.003	3279	3284	3293	rVB	49629	84581	3.08%	0.384%
20	21.462	3357	3362	3369	rVB3	25530	46626	1.70%	0.212%
21	21.997	3448	3453	3460	rVB3	24238	49923	1.82%	0.227%

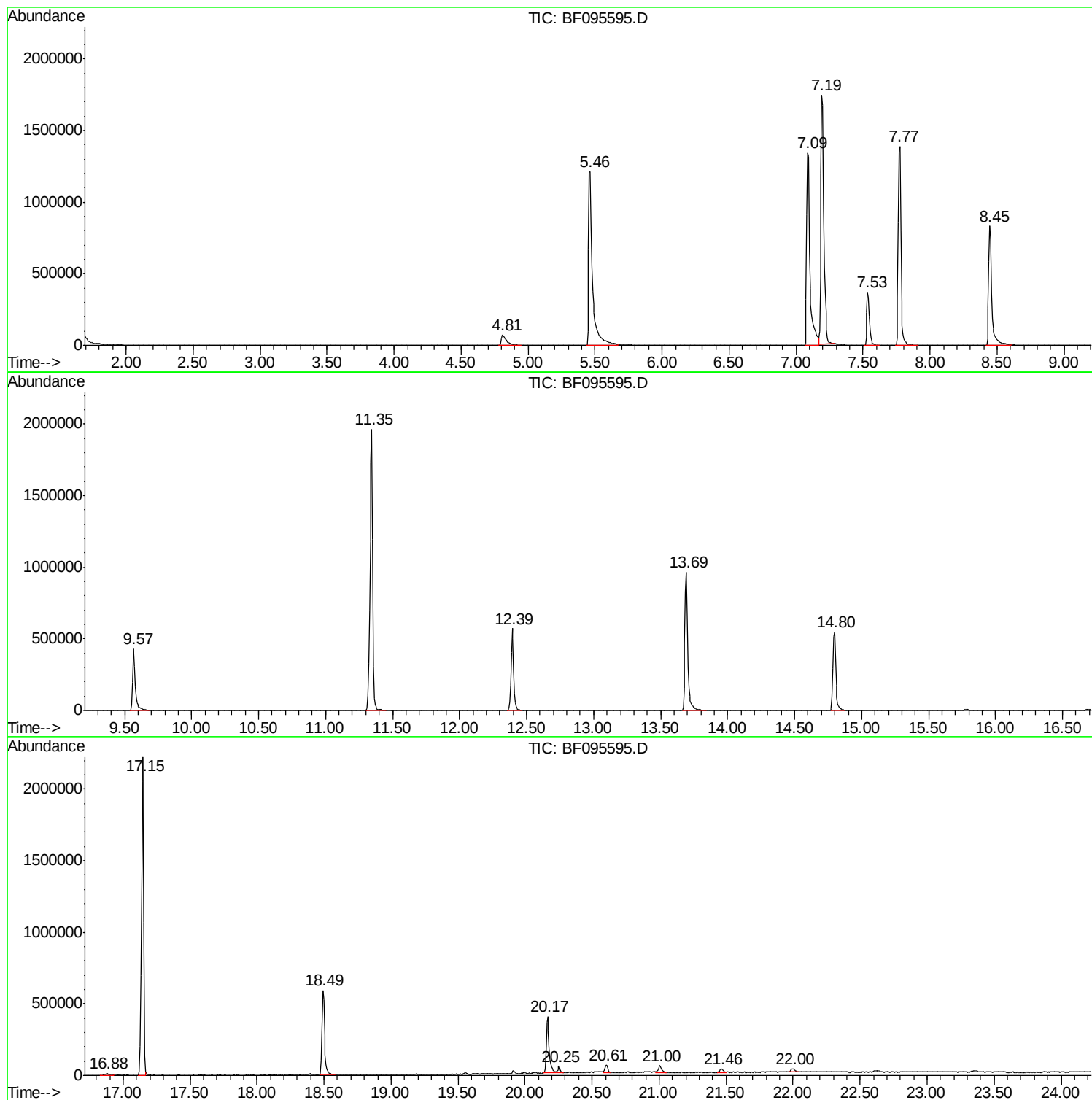
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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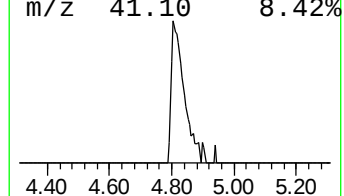
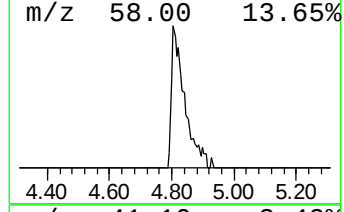
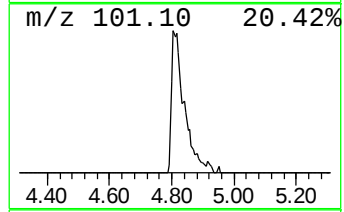
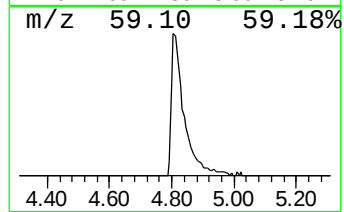
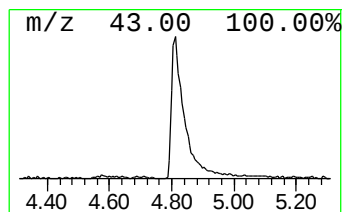
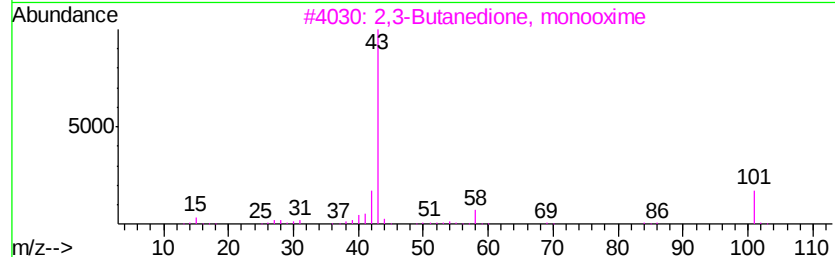
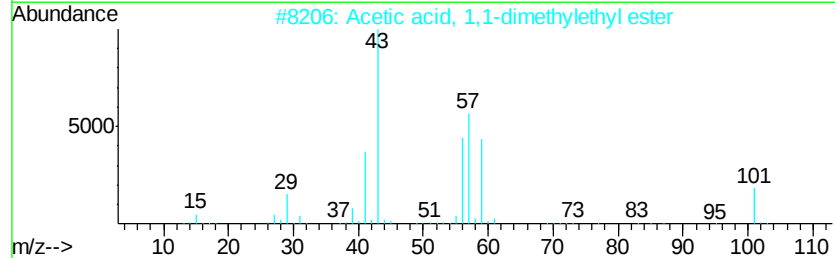
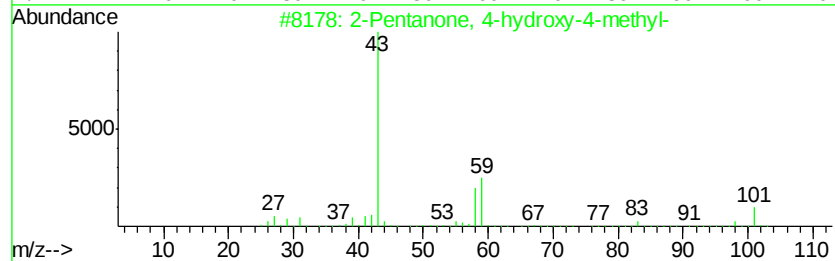
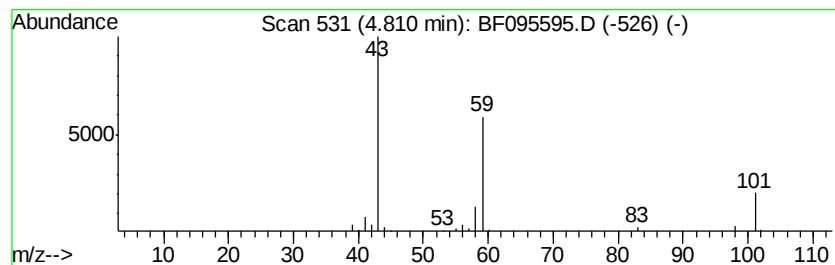
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	8.43 ng	210318	1,4-Dichlorobenzene-d4	7.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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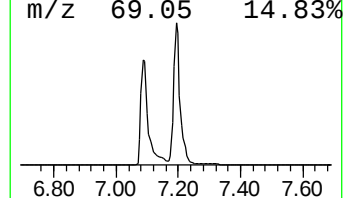
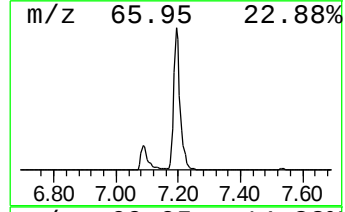
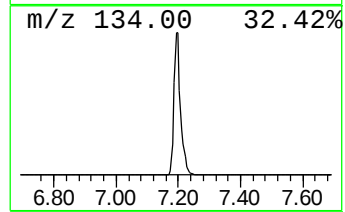
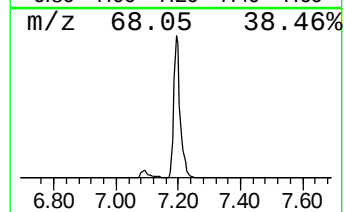
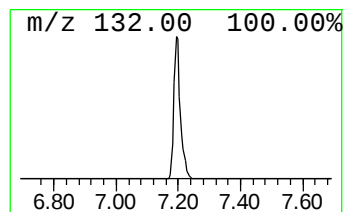
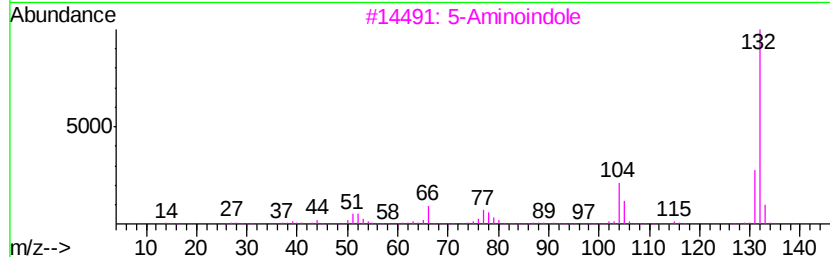
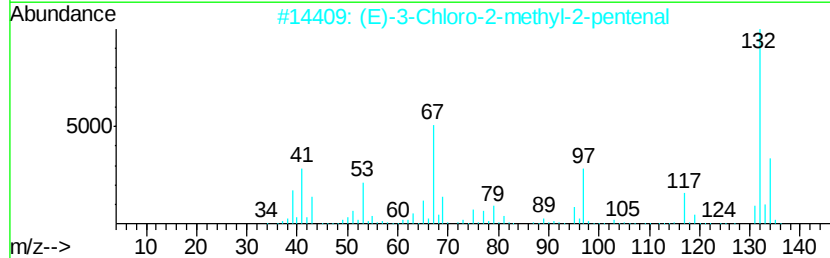
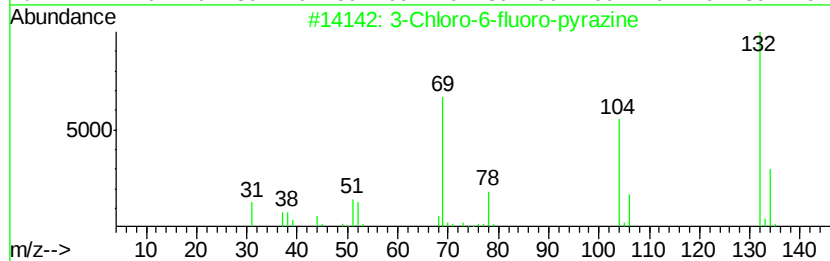
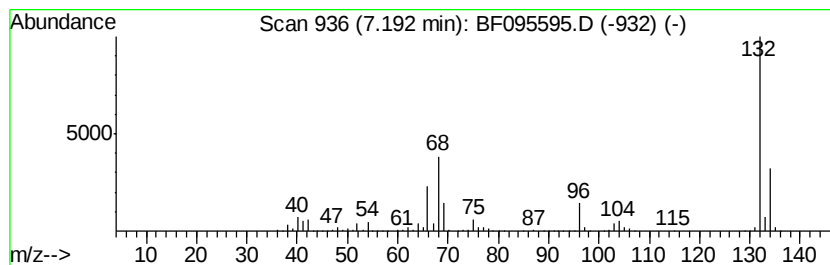
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	105.37 ng	2629200	1,4-Dichlorobenzene-d4	7.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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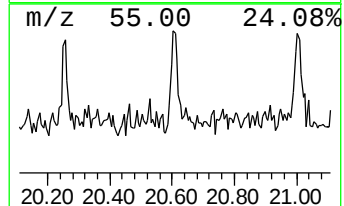
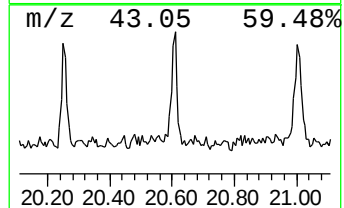
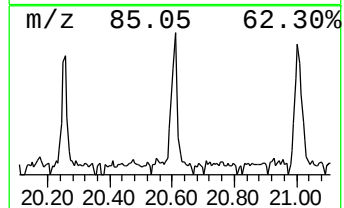
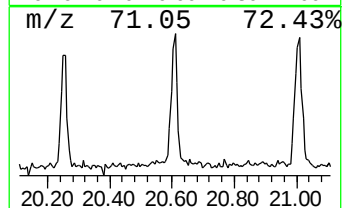
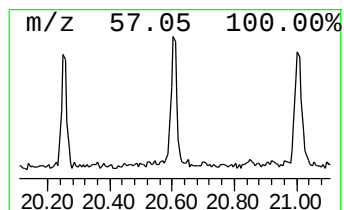
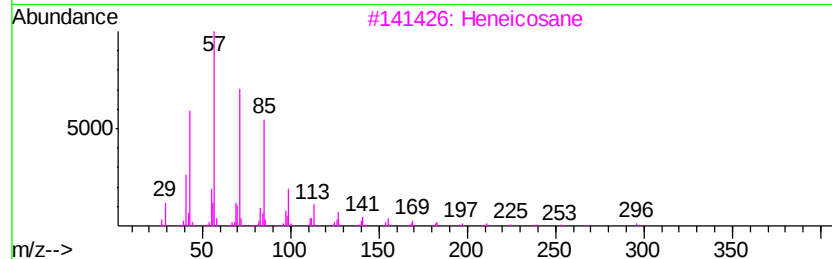
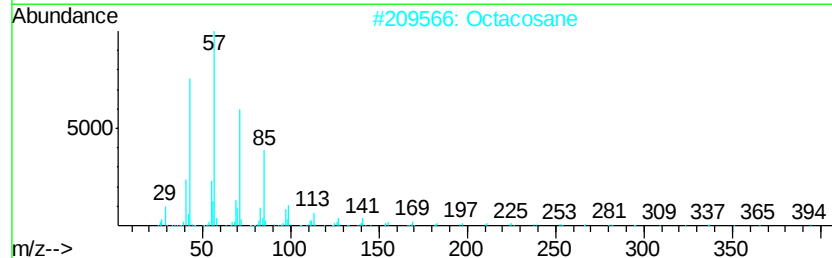
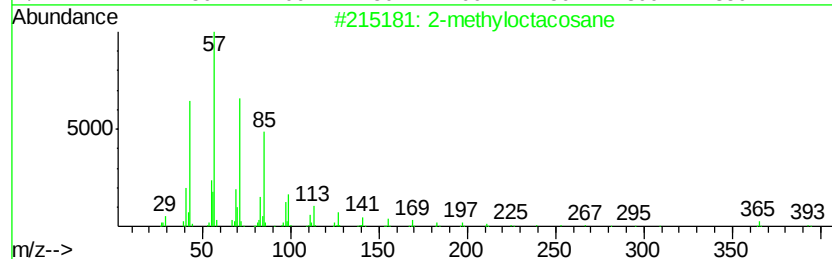
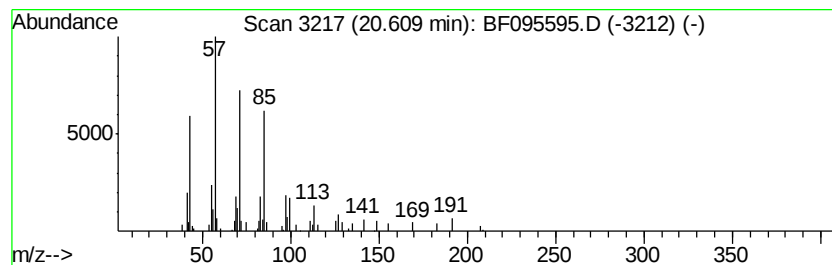
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Peak Number 4 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.61	2.18 ng	65564	Perylene-d12	20.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Octacosane	394	C28H58	000630-02-4	90
3		Heneicosane	296	C21H44	000629-94-7	87
4		Triacontane	422	C30H62	000638-68-6	86
5		Pentacosane	352	C25H52	000629-99-2	86



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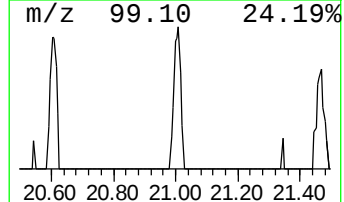
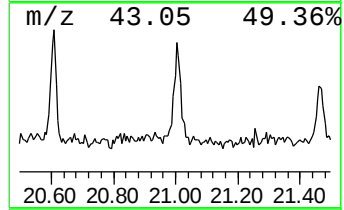
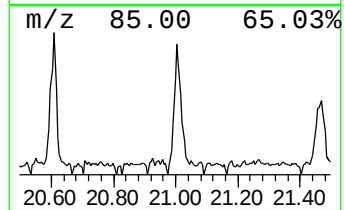
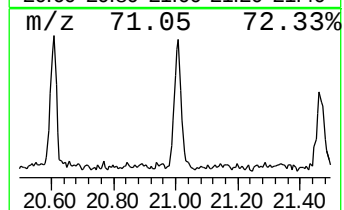
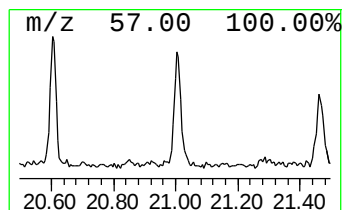
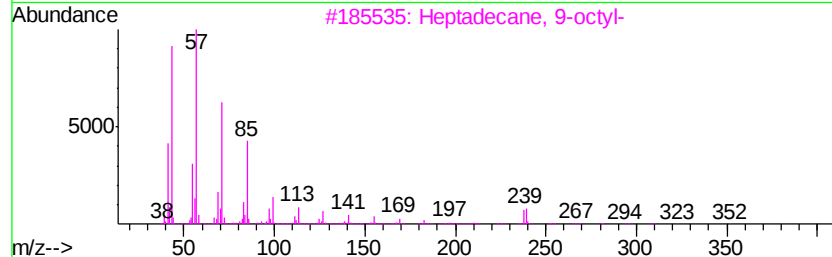
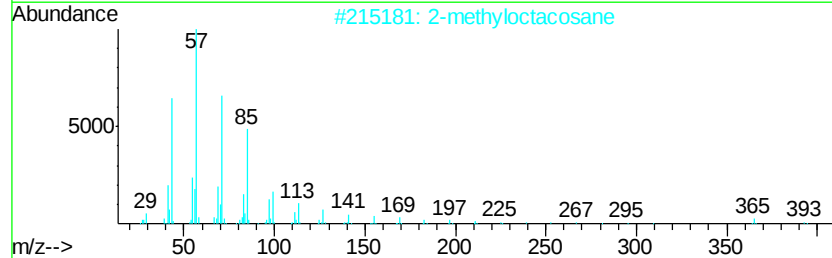
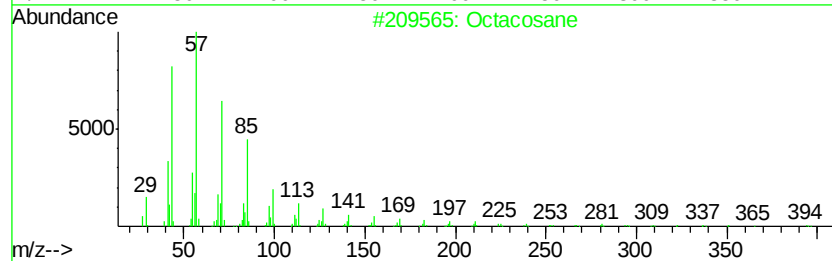
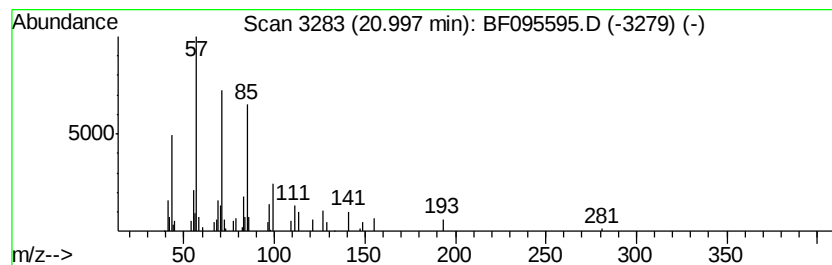
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Peak Number 5 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.00	2.81 ng	84581	Perylene-d12	20.17
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octacosane	394	C28H58	000630-02-4 91
2	2-methyloctacosane	408	C29H60	1000376-72-8 90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1 90
4	triacontane	422	C30H62	000638-68-6 90
5	Hexacosane	366	C26H54	000630-01-3 87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.81	8.4	ng	210318	1	7.53	499067	20.0
unknown7.19	7.19	105.4	ng	2629200	1	7.53	499067	20.0
2-methyloctacosane	20.61	2.2	ng	65564	6	20.17	602124	20.0
Octacosane	21.00	2.8	ng	84581	6	20.17	602124	20.0