

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082118\
 Data File : BF108329.D
 Acq On : 21 Aug 2018 10:50
 Operator : JU/SJ
 Sample : J4500-20
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-12

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-BF080818.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	3.213	144	149	155	rVB	61314	87987	1.22%	0.170%
2	5.278	495	500	512	rVB	702883	1006159	13.98%	1.943%
3	5.654	558	564	567	rBV	4538701	4954870	68.83%	9.569%
4	6.636	725	731	734	rBV	4343215	4595841	63.84%	8.876%
5	6.784	750	756	759	rBV	5424700	5491898	76.29%	10.606%
6	7.007	790	794	797	rBV	1390689	1101386	15.30%	2.127%
7	7.166	816	821	824	rBV	4682566	4243651	58.95%	8.196%
8	7.572	884	890	893	rBV	3489474	3819735	53.06%	7.377%
9	8.289	1007	1012	1014	rBV	1465956	1397341	19.41%	2.699%
10	8.307	1014	1015	1019	rVB	163059	114823	1.60%	0.222%
11	9.366	1189	1195	1198	rBV	6503071	6591121	91.56%	12.729%
12	10.048	1306	1311	1315	rBV	1660584	1621130	22.52%	3.131%
13	10.848	1440	1447	1450	rBV	4347520	4533667	62.98%	8.756%
14	11.548	1560	1566	1569	rBV	2089801	1752697	24.35%	3.385%
15	13.142	1831	1837	1840	rBV	6469205	7198923	100.00%	13.903%
16	14.201	2013	2017	2020	rBV	1624288	1393059	19.35%	2.690%
17	14.636	2083	2091	2097	rBV2	74100	115153	1.60%	0.222%
18	14.959	2143	2146	2152	rVB	69127	81123	1.13%	0.157%
19	15.324	2204	2208	2214	rVB	95361	119265	1.66%	0.230%
20	15.759	2274	2282	2289	rVB	687100	1114564	15.48%	2.153%
21	16.218	2354	2360	2366	rVB	119362	204318	2.84%	0.395%
22	16.771	2448	2454	2461	rVB	85440	162197	2.25%	0.313%
23	17.424	2560	2565	2572	rVB3	37663	78524	1.09%	0.152%

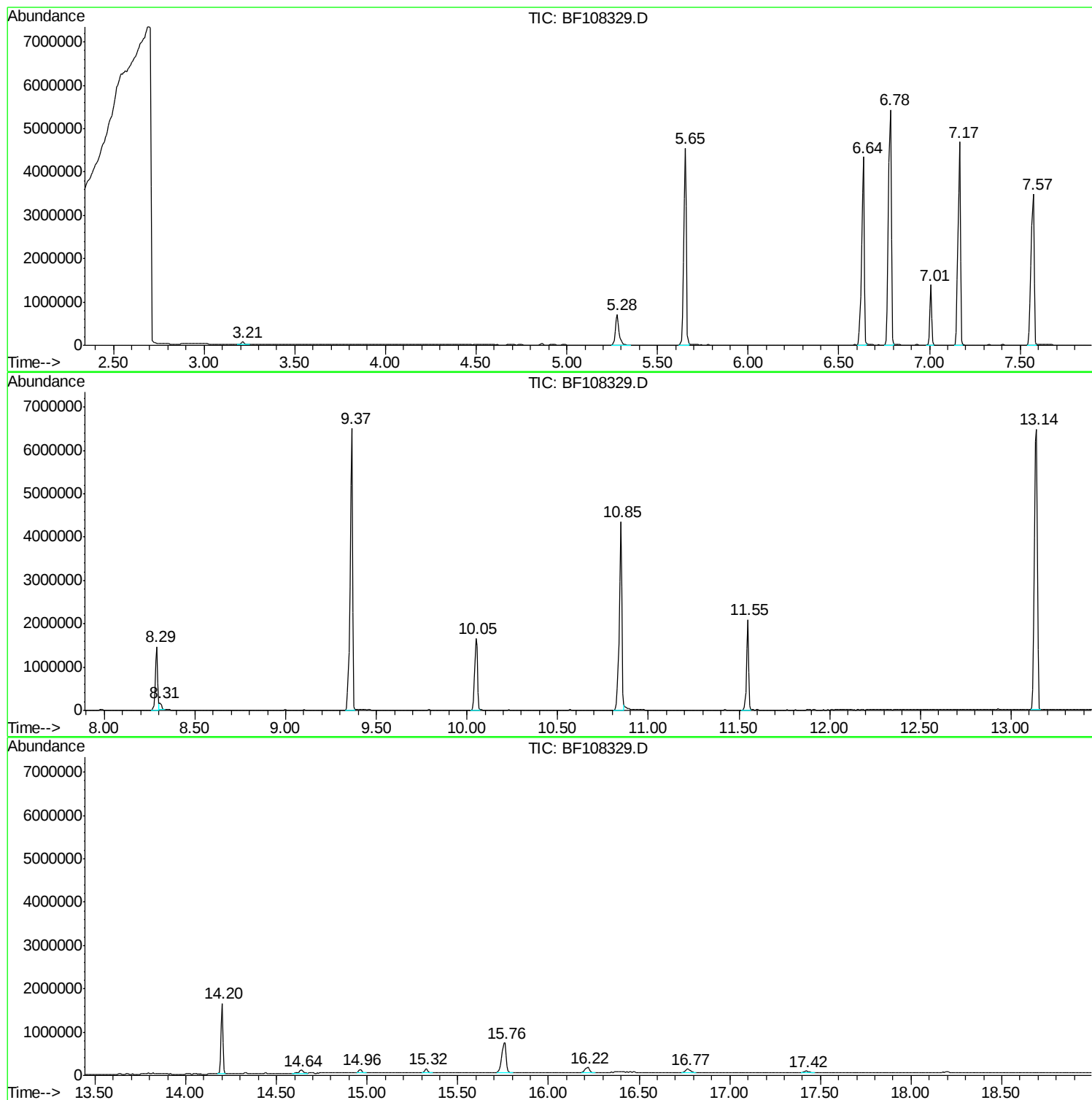
Sum of corrected areas: 51779432

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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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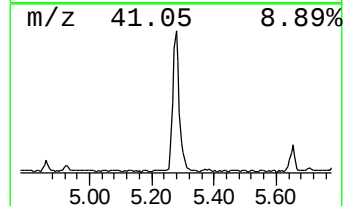
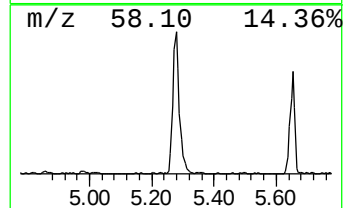
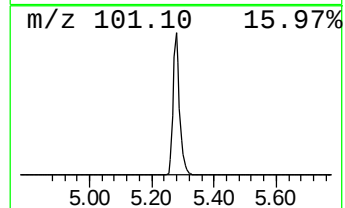
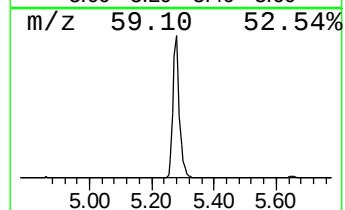
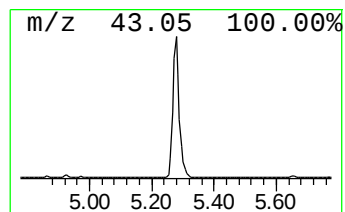
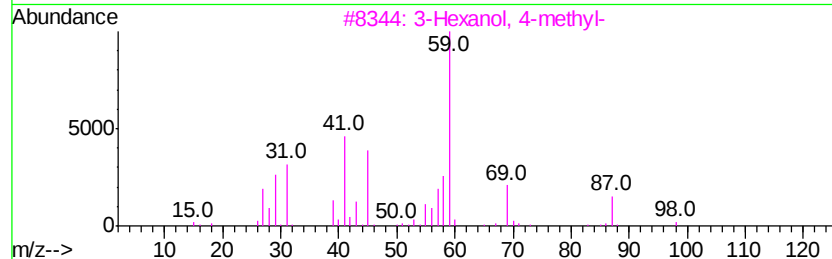
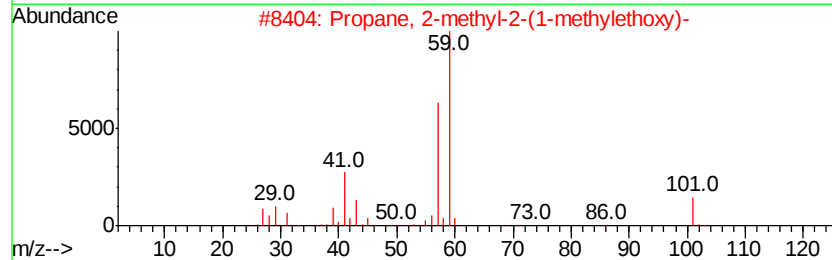
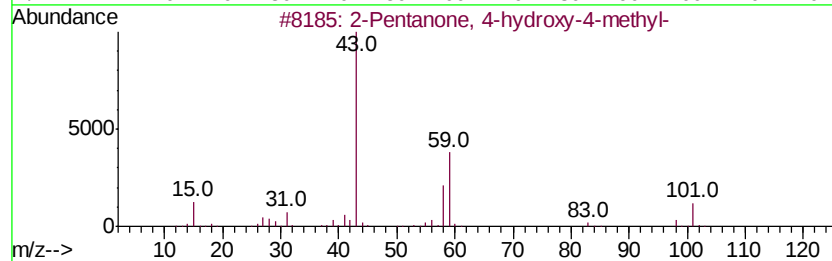
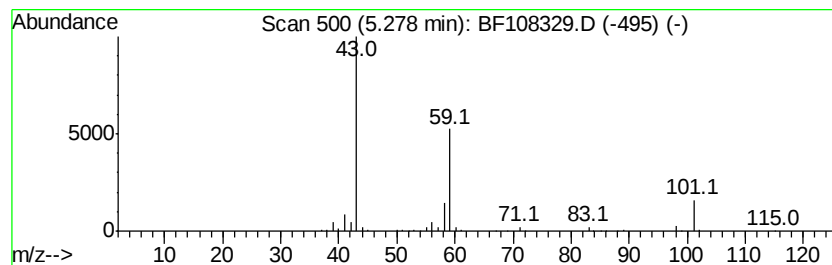
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.28	18.27 ng	1006160	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	42
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25



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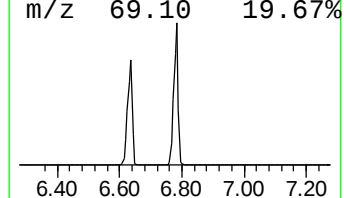
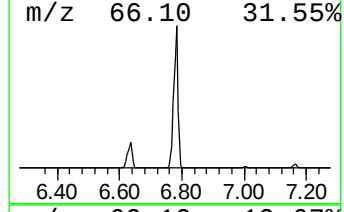
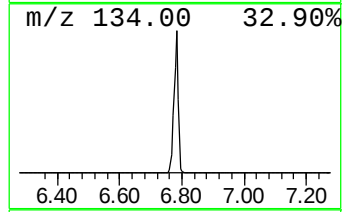
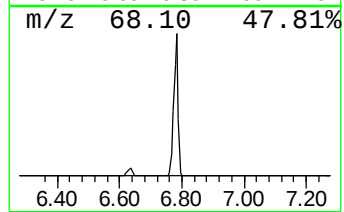
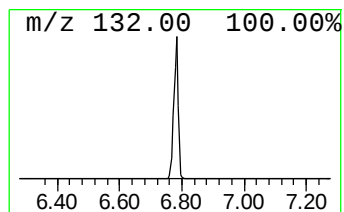
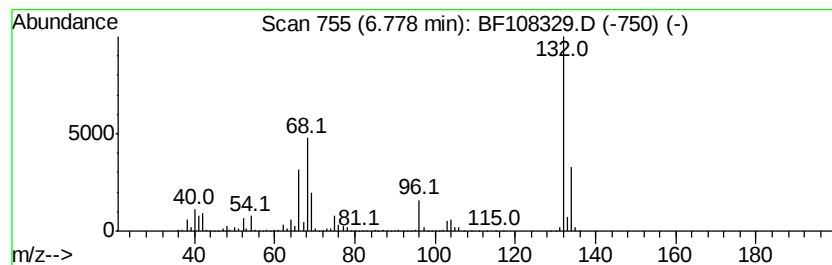
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	99.73 ng	5491900	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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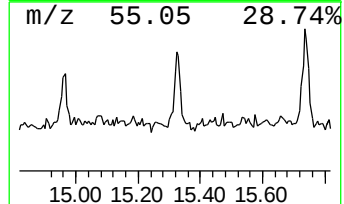
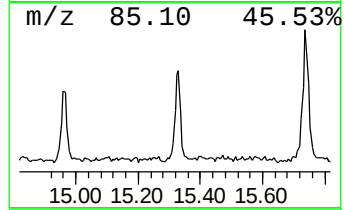
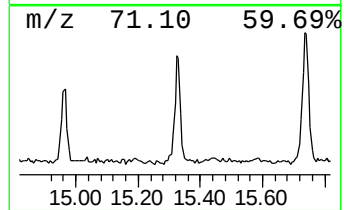
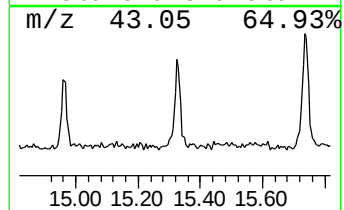
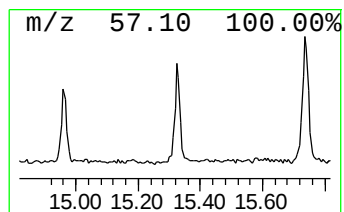
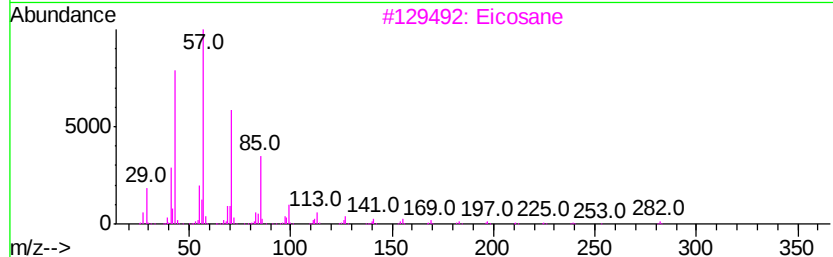
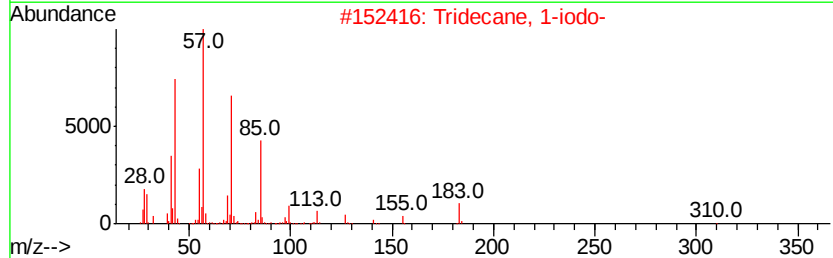
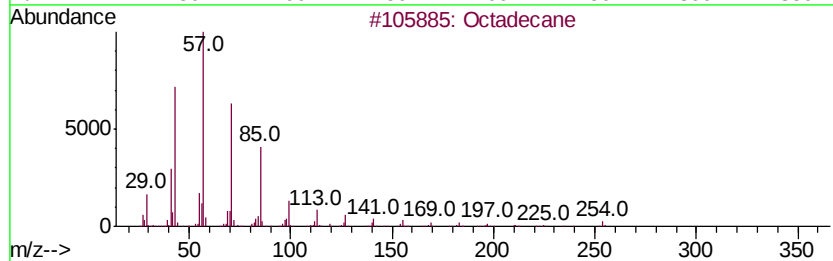
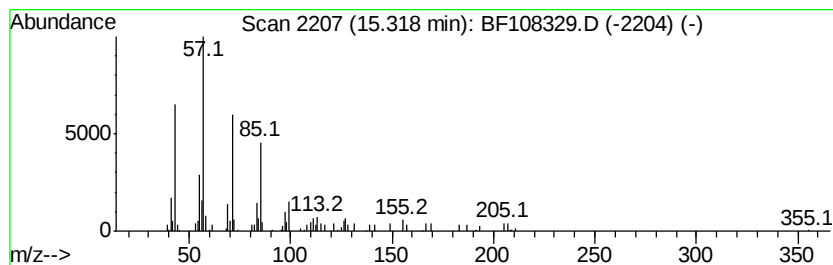
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Peak Number 4 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	2.14 ng	119265	Perylene-d12	15.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	91
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
3		Eicosane	282	C20H42	000112-95-8	91
4		Tetracosane	338	C24H50	000646-31-1	90
5		Octacosane	394	C28H58	000630-02-4	90



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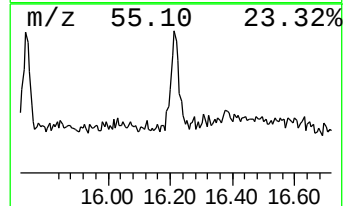
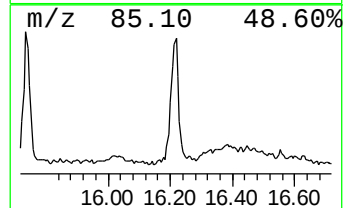
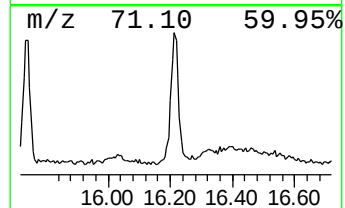
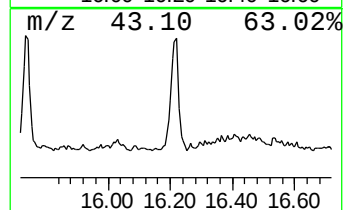
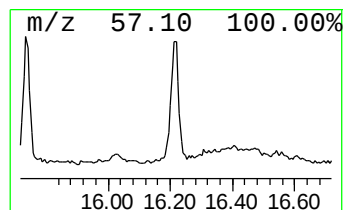
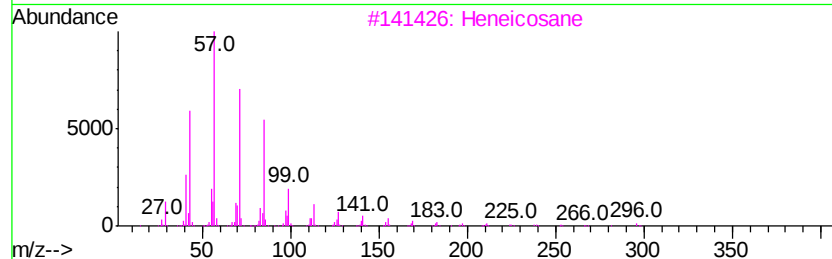
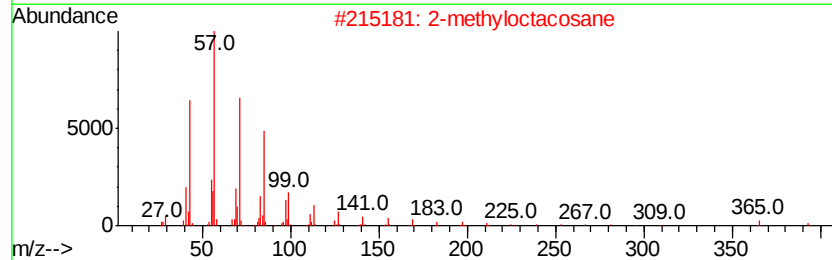
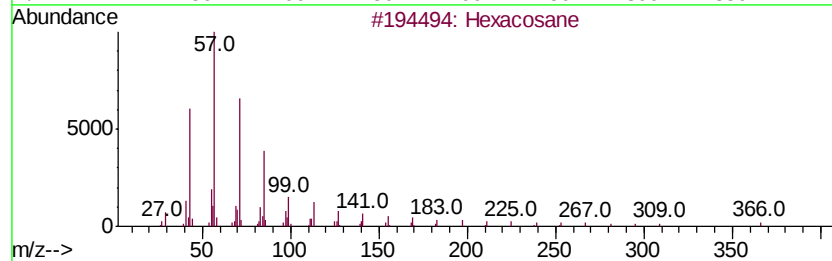
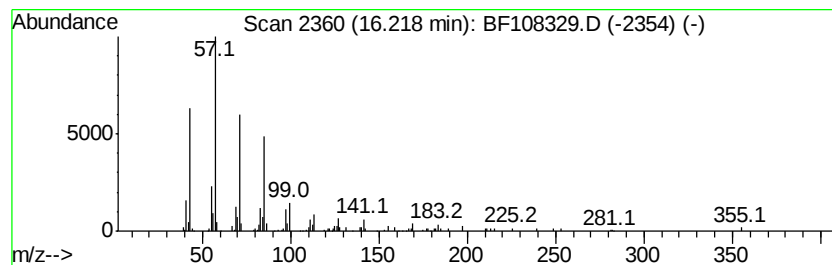
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 Peak Number 5 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.22	3.67 ng	204318	Perylene-d12	15.76	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Docosane	310	C22H46	000629-97-0	87
5	Octacosane	394	C28H58	000630-02-4	87



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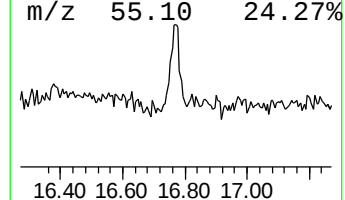
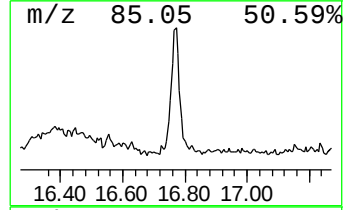
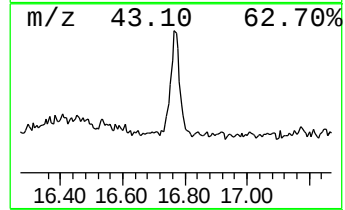
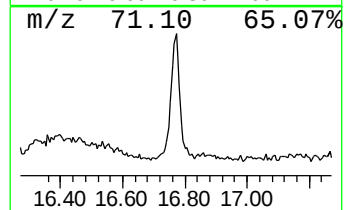
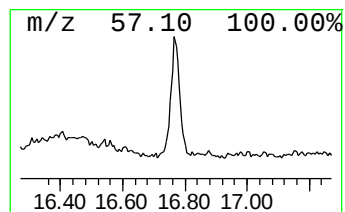
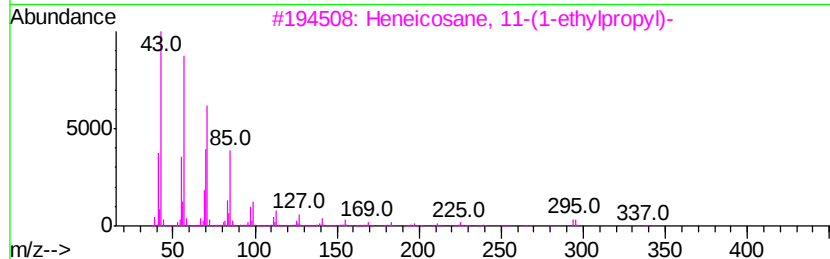
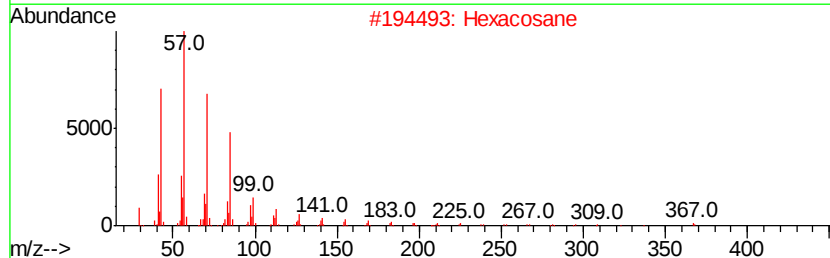
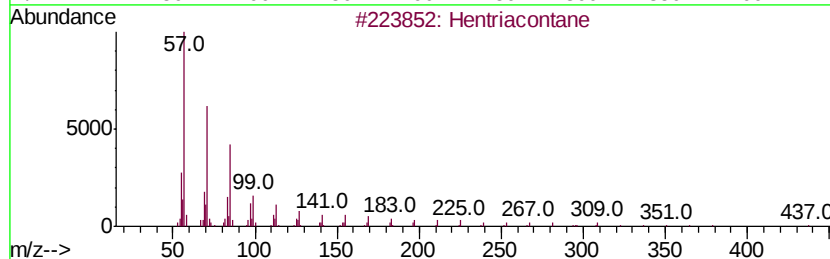
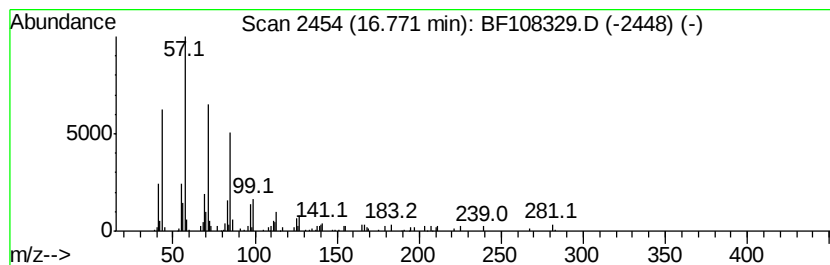
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Peak Number 6 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.77	2.91 ng	162197	Perylene-d12	15.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	90
5	Tetratetracontane		619	C44H90	007098-22-8	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.28	18.3	ng	1006160	1	7.01	1101390	20.0
unknown6.78	6.78	99.7	ng	5491900	1	7.01	1101390	20.0
Octadecane	15.32	2.1	ng	119265	6	15.76	1114560	20.0
Hexacosane	16.22	3.7	ng	204318	6	15.76	1114560	20.0
Hentriacontane	16.77	2.9	ng	162197	6	15.76	1114560	20.0