

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
 Data File : BF096584.D
 Acq On : 8 Jul 2017 2:56
 Operator : SJ/MA
 Sample : I4095-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-011

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-BF070117.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	4.881	470	475	482	rBV	293547	349409	18.96%	2.117%
2	5.310	543	548	551	rBV	1960120	1804019	97.87%	10.928%
3	6.339	718	723	729	rBV	1774778	1843299	100.00%	11.166%
4	6.469	740	745	748	rBV	1958769	1764732	95.74%	10.690%
5	6.698	780	784	788	rBV	704921	559682	30.36%	3.390%
6	6.857	806	811	814	rBV	1487124	1293542	70.18%	7.836%
7	7.257	874	879	882	rBV	1208643	1014801	55.05%	6.147%
8	7.981	998	1002	1005	rBV	879016	712348	38.65%	4.315%
9	9.057	1180	1185	1188	rBV	2048818	1740959	94.45%	10.546%
10	9.451	1248	1252	1255	rBV	190867	163690	8.88%	0.992%
11	9.628	1279	1282	1288	rBV3	17863	29450	1.60%	0.178%
12	9.733	1296	1300	1304	rVB	796619	721513	39.14%	4.371%
13	10.145	1359	1370	1372	rBV	17112	23994	1.30%	0.145%
14	10.175	1372	1375	1379	rVB	26860	23110	1.25%	0.140%
15	10.516	1429	1433	1436	rBV	1078305	922330	50.04%	5.587%
16	10.645	1453	1455	1462	rVB	36898	45209	2.45%	0.274%
17	11.098	1528	1532	1534	rBV2	27701	28388	1.54%	0.172%
18	11.210	1547	1551	1555	rBV	778270	639887	34.71%	3.876%
19	12.792	1816	1820	1824	rBV	1461985	1294443	70.22%	7.841%
20	13.698	1970	1974	1980	rBV	143930	163894	8.89%	0.993%
21	13.839	1994	1998	2002	rBV	619051	551278	29.91%	3.339%
22	14.333	2079	2082	2086	rBV3	36395	38101	2.07%	0.231%
23	15.239	2232	2236	2241	rBV	296597	372668	20.22%	2.258%
24	19.039	2876	2882	2891	rVB8	149324	407176	22.09%	2.467%

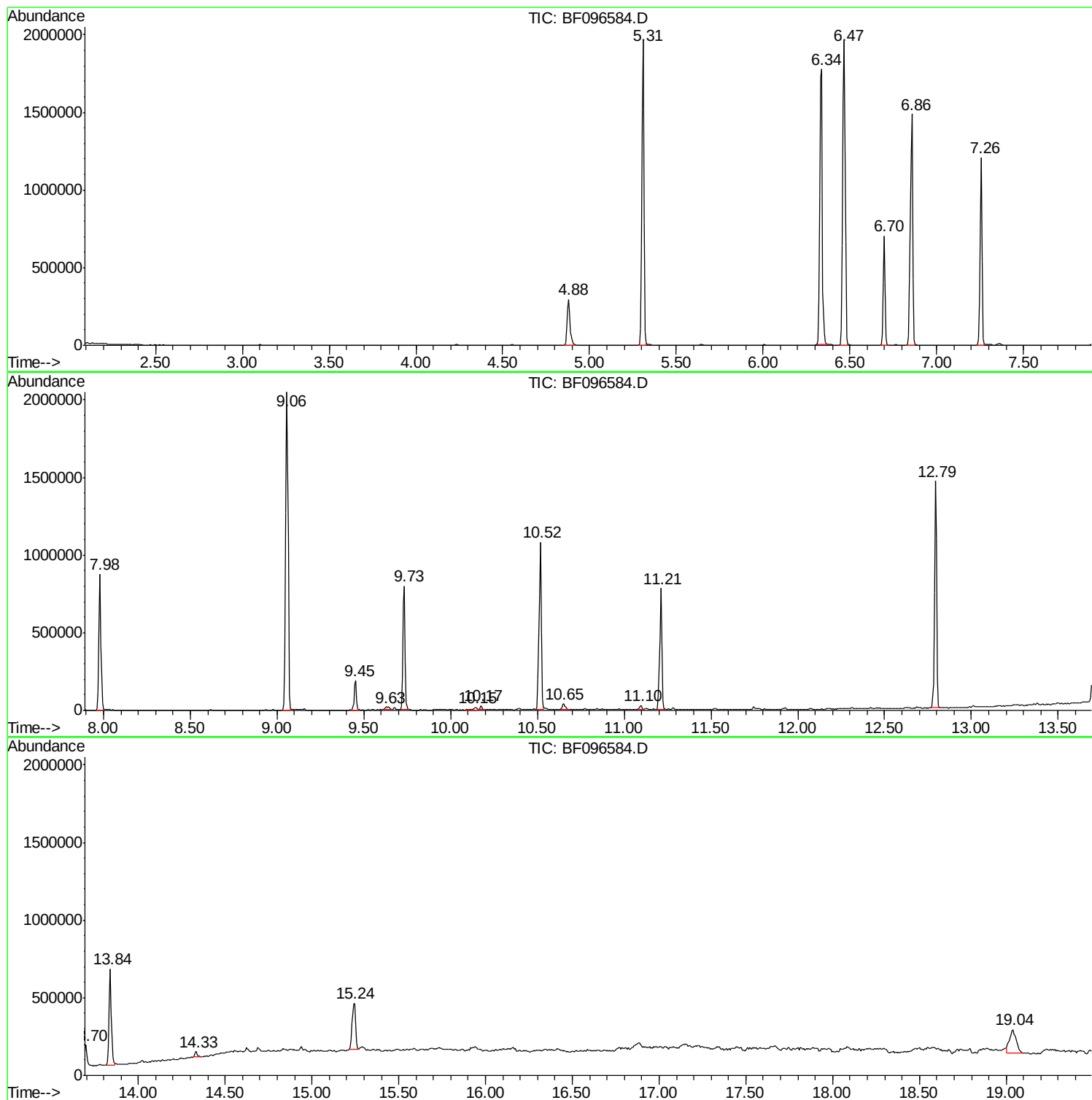
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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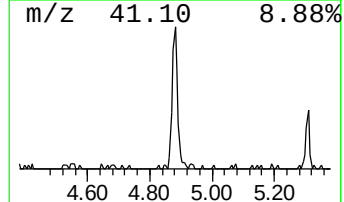
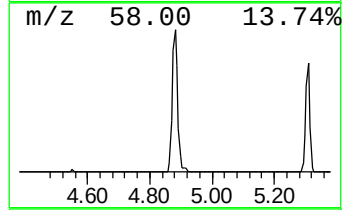
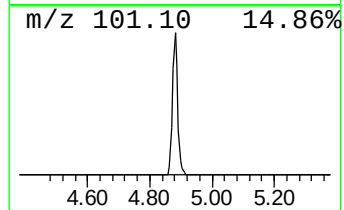
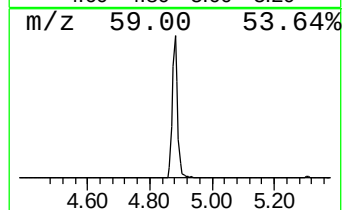
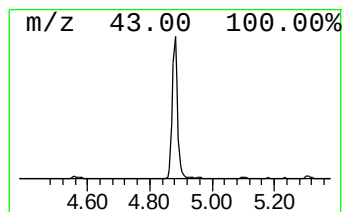
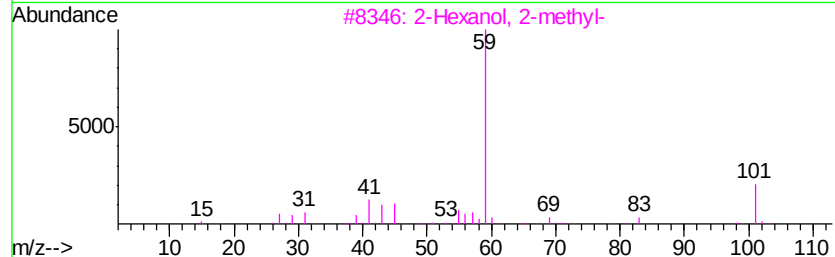
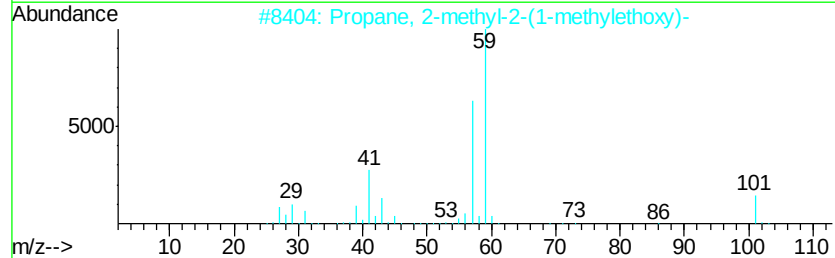
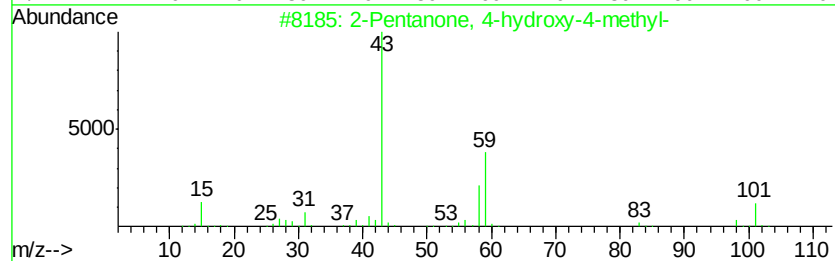
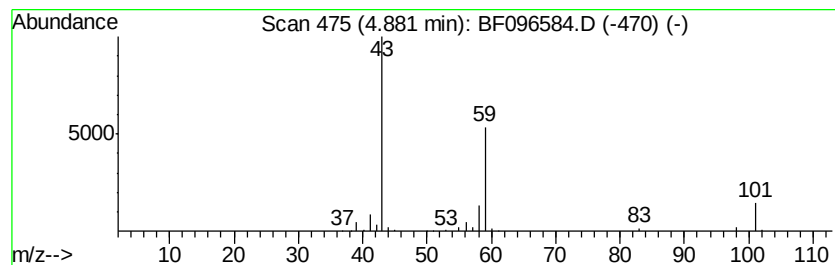
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	12.49 ng	349409	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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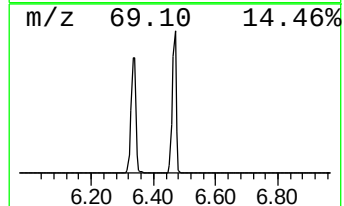
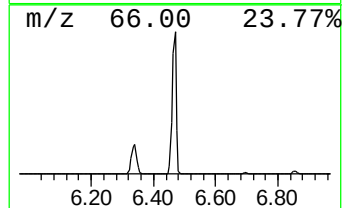
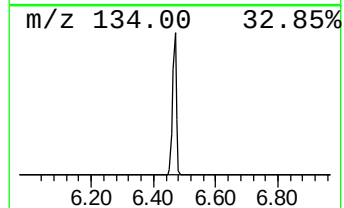
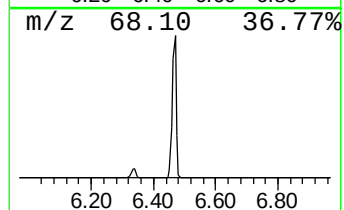
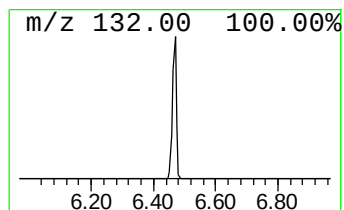
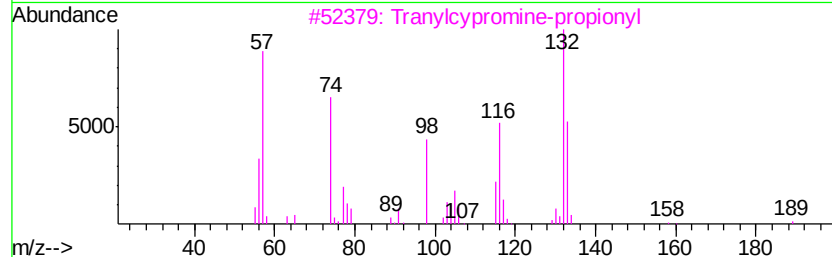
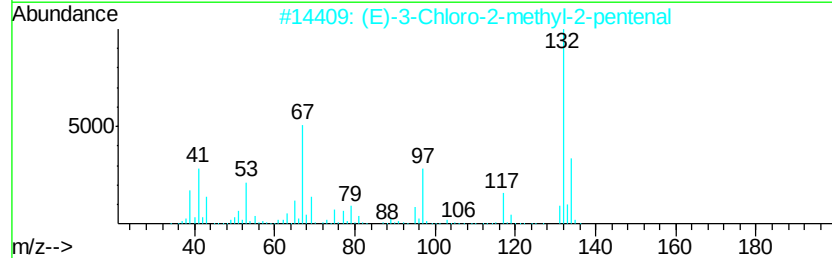
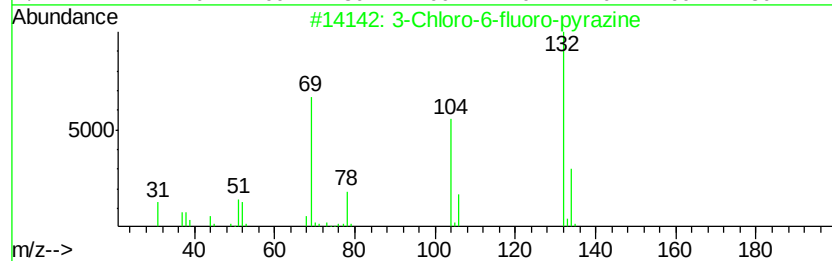
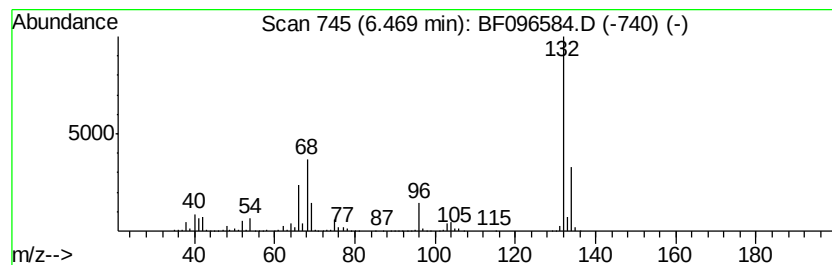
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	63.06 ng	1764730	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	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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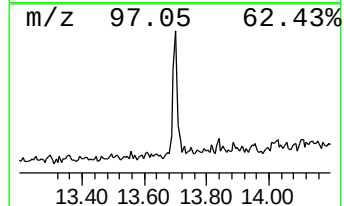
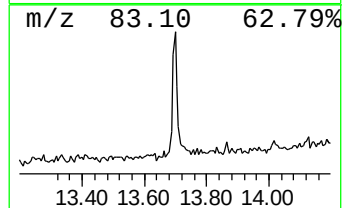
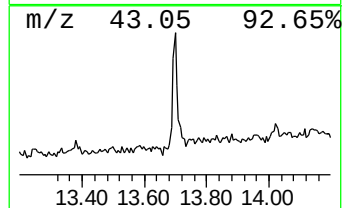
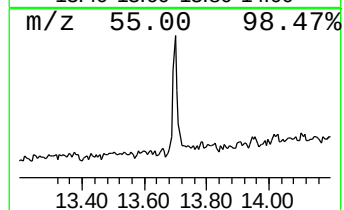
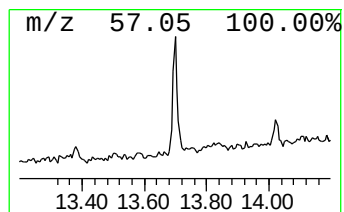
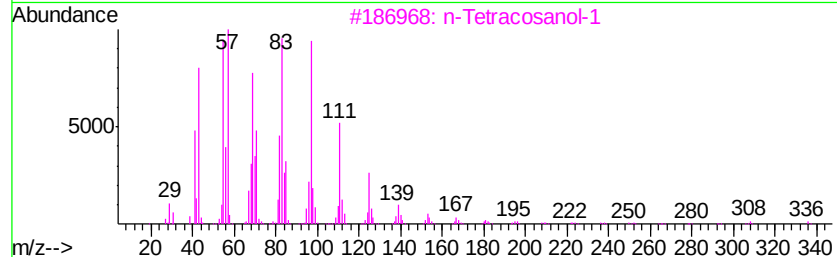
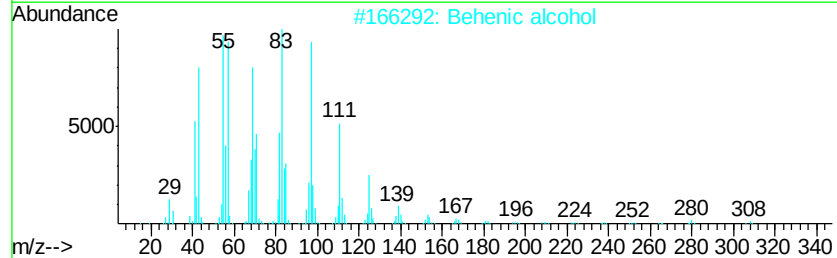
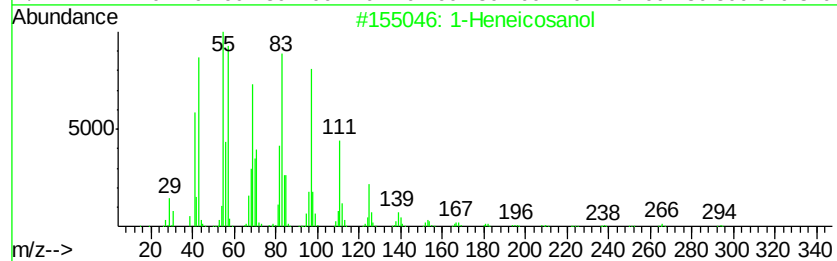
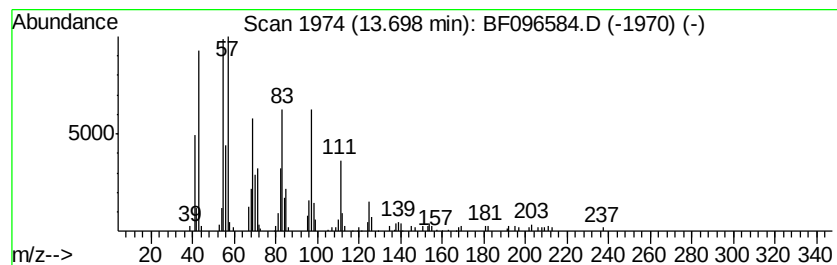
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Peak Number 4 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	5.95 ng	163894	Chrysene-d12	13.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	93
2		Behenic alcohol	326	C22H46O	000661-19-8	93
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4		1-Octadecanol	270	C18H38O	000112-92-5	91
5		1-Nonadecene	266	C19H38	018435-45-5	90



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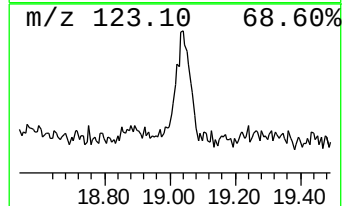
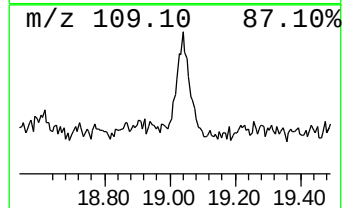
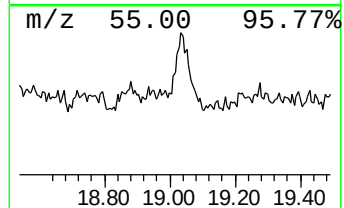
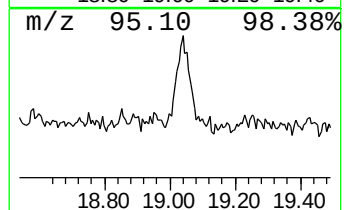
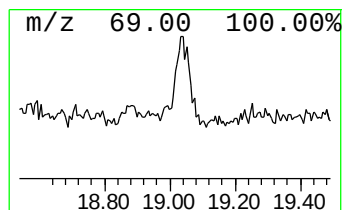
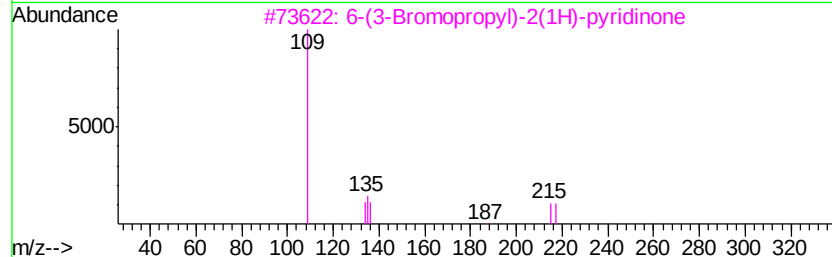
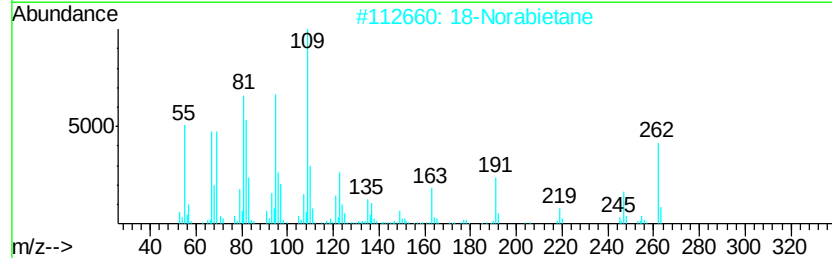
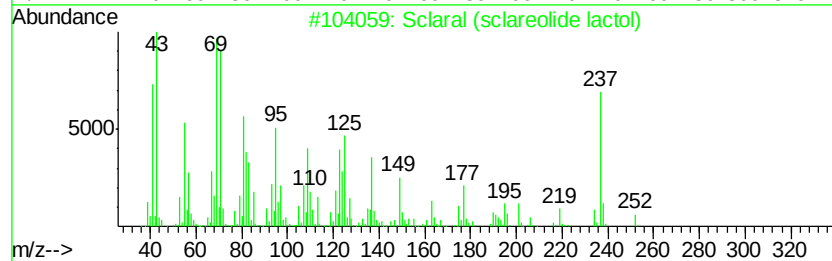
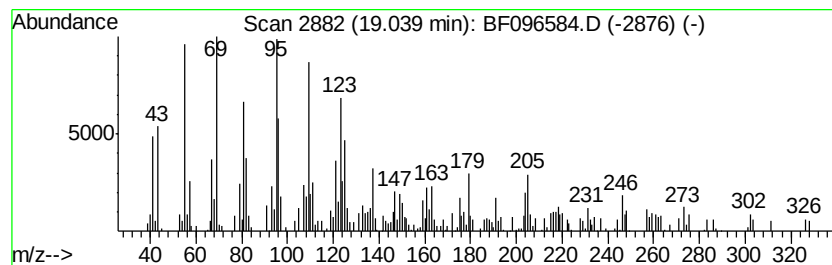
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Peak Number 5 unknown19.04 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.04	21.85 ng	407176	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Scleral (sclareolide lactol)	252	C16H28O2	052811-62-8	43
2		18-Norabietane	262	C19H34	1000293-16-6	38
3		6-(3-Bromopropyl)-2(1H)-pyridinone	215	C8H10BrN0	101773-69-7	30
4		1-Isopropoxy-2-trifluoroacetox...	248	C11H11F3O3	1000278-65-1	30
5		Imidazole, 4-methyl-5-[3,3,3-tri...	234	C10H13F3N2O	1000129-15-8	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.88	12.5	ng	349409	1	6.70	559682	20.0
unknown6.47	6.47	63.1	ng	1764730	1	6.70	559682	20.0
1-Heneicosanol	13.70	6.0	ng	163894	5	13.84	551278	20.0
unknown19.04	19.04	21.9	ng	407176	6	15.24	372668	20.0