

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051617\
 Data File : BF095168.D
 Acq On : 16 May 2017 21:34
 Operator : SJ/MA
 Sample : I3160-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-WC-4

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:\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	5.148	542	546	566	rBV	221035	483752	14.01%	1.863%
2	5.748	644	648	680	rBV	1557676	2788120	80.76%	10.739%
3	7.325	910	916	931	rBV	1749022	2706777	78.40%	10.426%
4	7.442	931	936	957	rVB	2208420	3075406	89.08%	11.845%
5	7.777	989	993	1008	rVB	517312	621708	18.01%	2.395%
6	8.013	1028	1033	1052	rBV	1863423	2320820	67.22%	8.939%
7	8.677	1140	1146	1161	rBV	1282174	1748444	50.65%	6.734%
8	9.789	1331	1335	1352	rBV	604610	843345	24.43%	3.248%
9	10.836	1508	1513	1521	rVB	333442	395617	11.46%	1.524%
10	11.295	1586	1591	1601	rBV2	70964	97733	2.83%	0.376%
11	11.565	1631	1637	1655	rBV	2653016	3452338	100.00%	13.297%
12	12.254	1749	1754	1764	rBV	327031	508369	14.73%	1.958%
13	12.336	1764	1768	1775	rVB	37307	46602	1.35%	0.179%
14	12.618	1811	1816	1834	rBV2	652988	927284	26.86%	3.572%
15	13.918	2031	2037	2057	rBV	1163366	1745355	50.56%	6.722%
16	14.224	2083	2089	2093	rBV	29277	36089	1.05%	0.139%
17	15.024	2220	2225	2250	rVB	511984	761439	22.06%	2.933%
18	15.983	2383	2388	2397	rBV4	40992	79555	2.30%	0.306%
19	17.342	2614	2619	2636	rBV	1977573	2346479	67.97%	9.038%
20	18.694	2845	2849	2864	rVB	339127	503188	14.58%	1.938%
21	20.365	3129	3133	3142	rBV	340401	474564	13.75%	1.828%

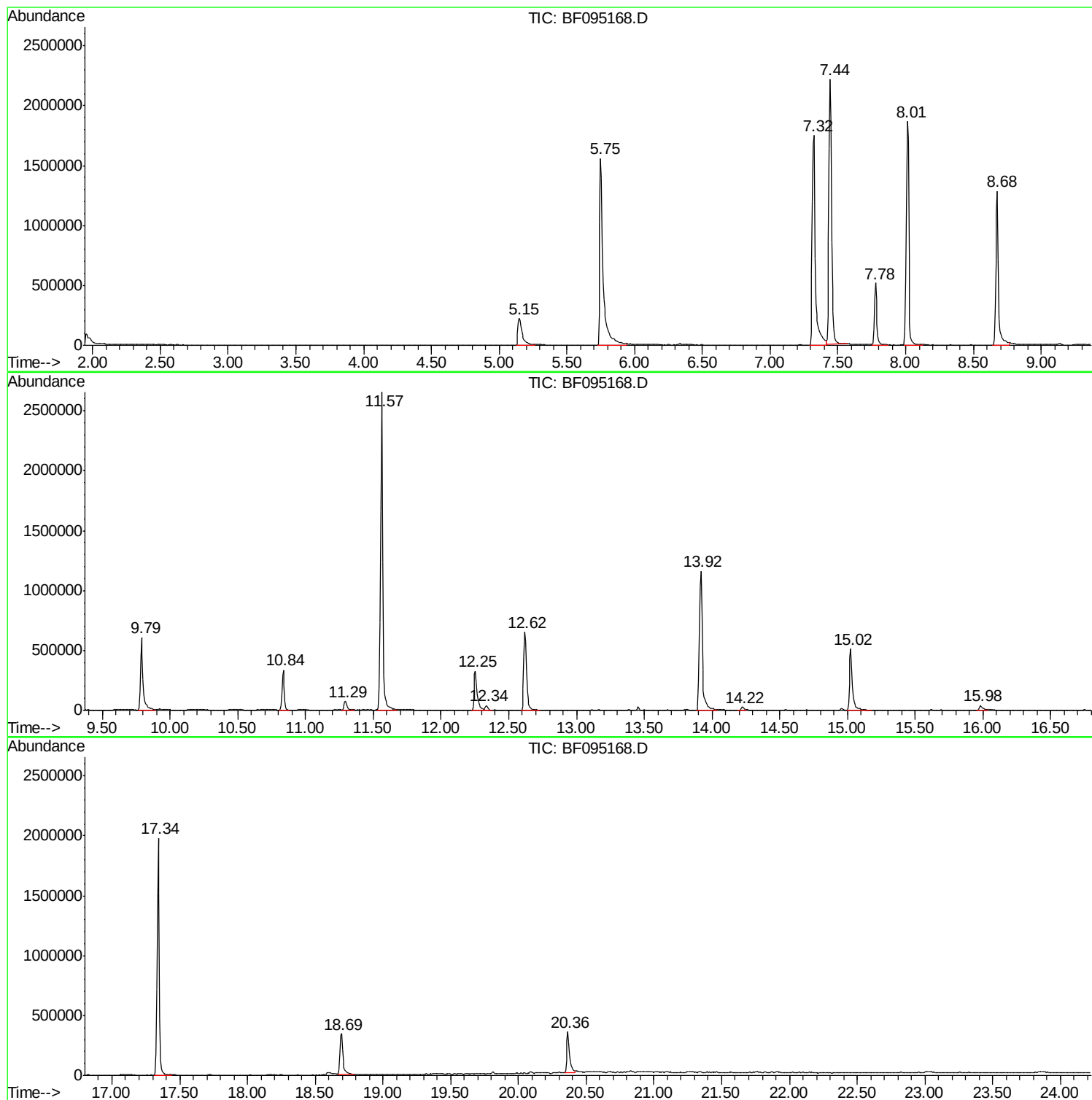
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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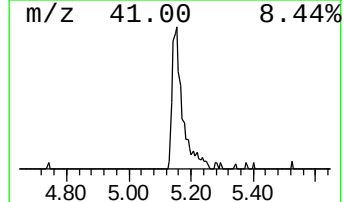
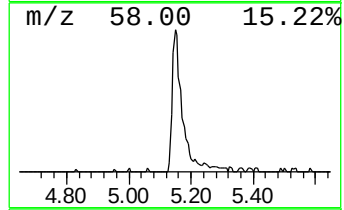
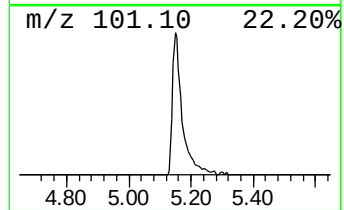
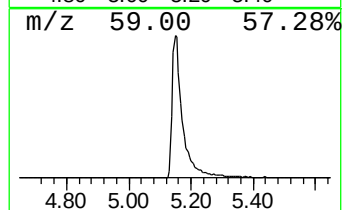
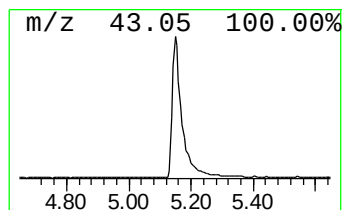
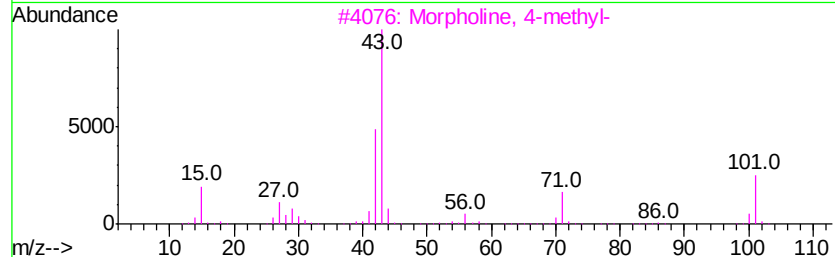
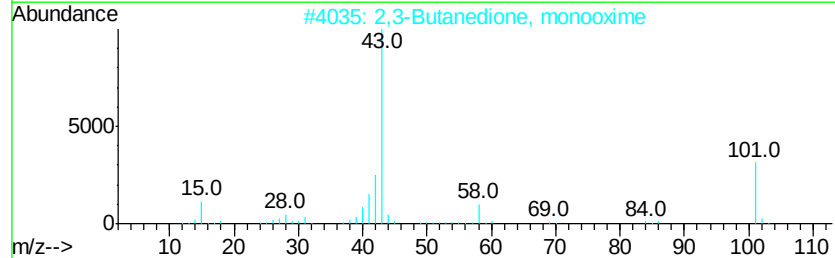
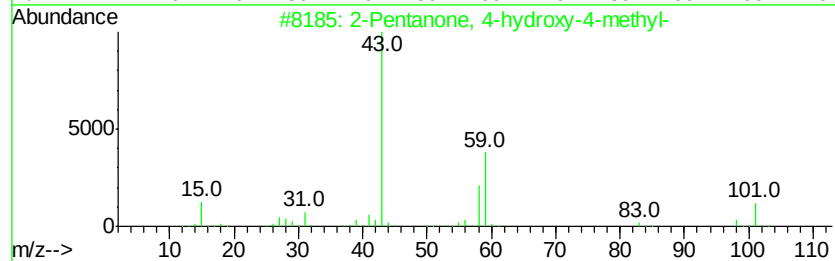
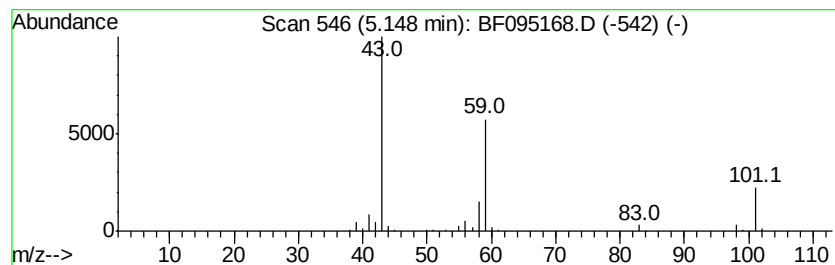
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.15	15.56 ng	483752	1,4-Dichlorobenzene-d4	7.78

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	17		
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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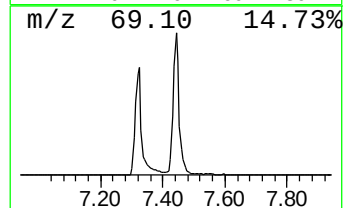
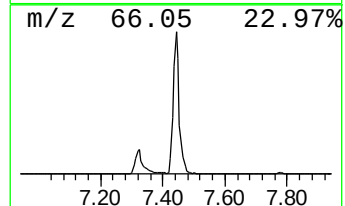
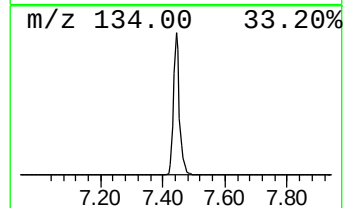
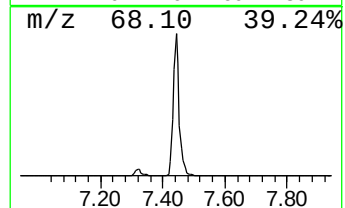
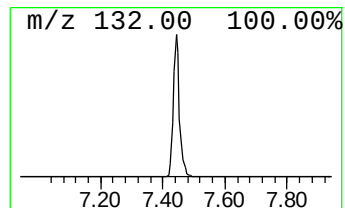
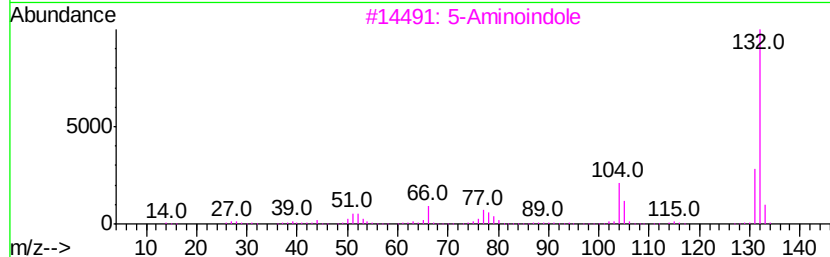
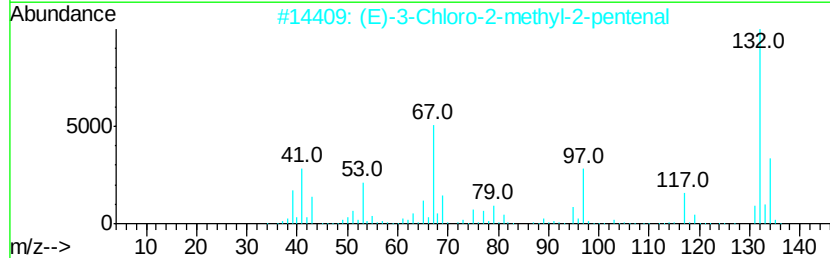
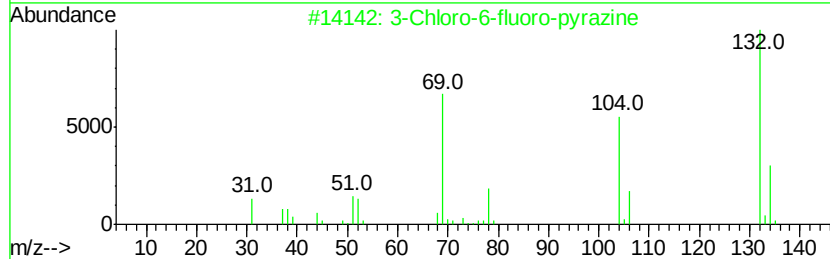
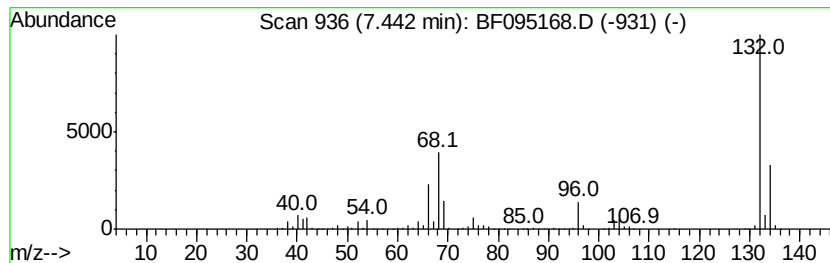
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Peak Number 2 unknown7.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	98.93 ng	3075410	1,4-Dichlorobenzene-d4	7.78

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		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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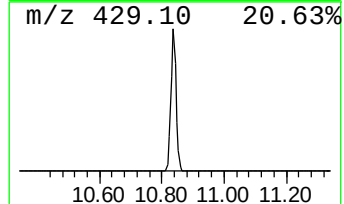
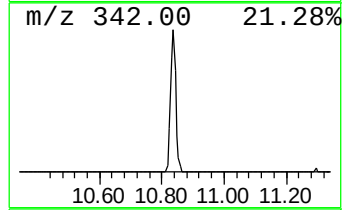
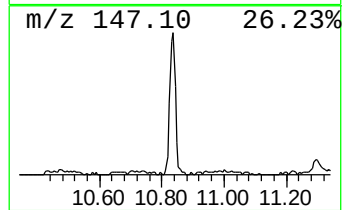
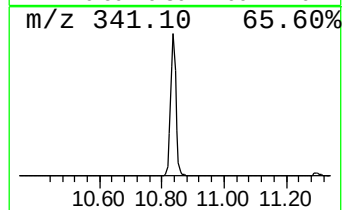
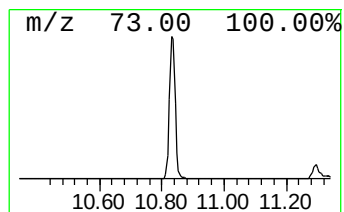
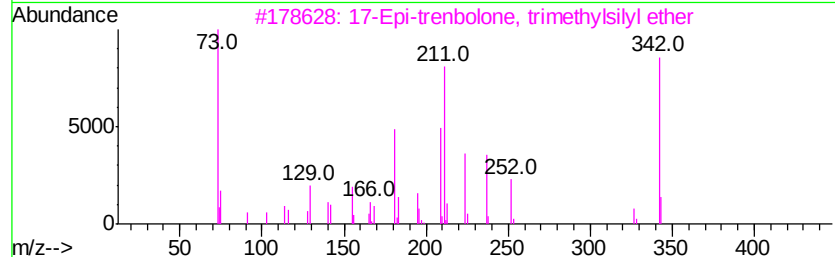
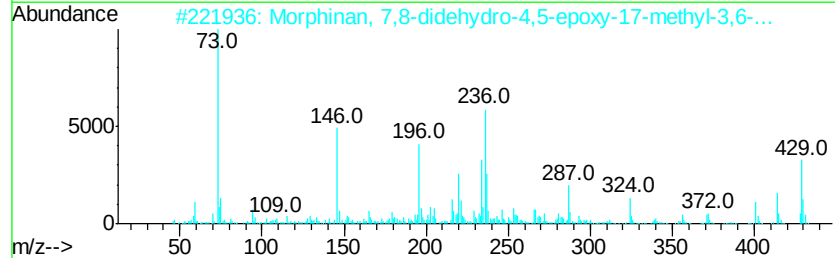
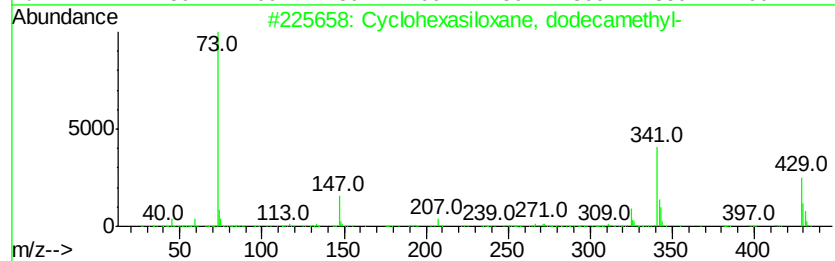
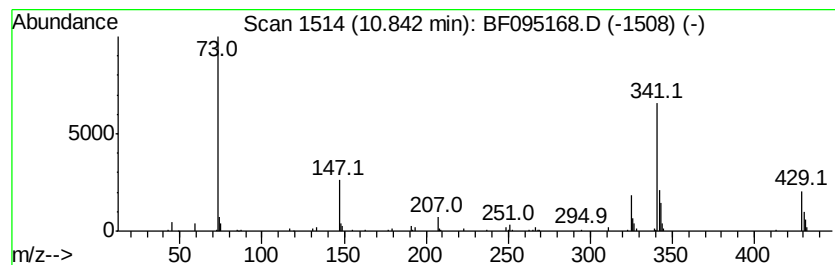
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Peak Number 4 Cyclohexasiloxane, dodecane... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.84	9.38 ng	395617	Naphthalene-d8	9.79		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	91
2		Morphinan, 7,8-didehydro-4,5-epo...	429	C23H35N03Si2	055449-66-6	18
3		17-Epi-trenbolone, trimethylsilyl...	342	C21H30O2Si	1000293-11-0	14
4		Benzene, 1,2,3-tris[(trimethylsilyl...	342	C15H30O3Si3	017864-23-2	10
5		Norcodeine di-TMS derivative	429	C23H35N03Si2	1000137-11-3	9



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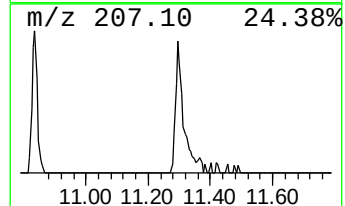
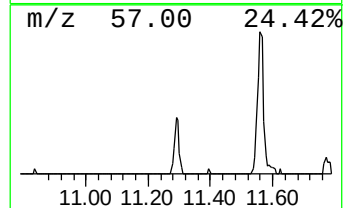
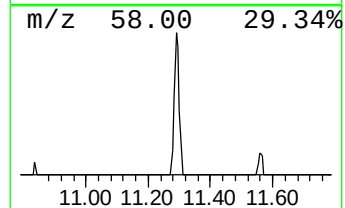
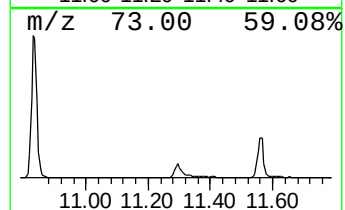
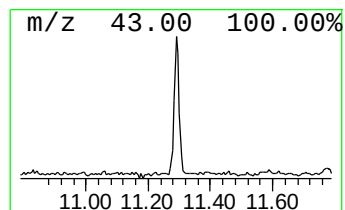
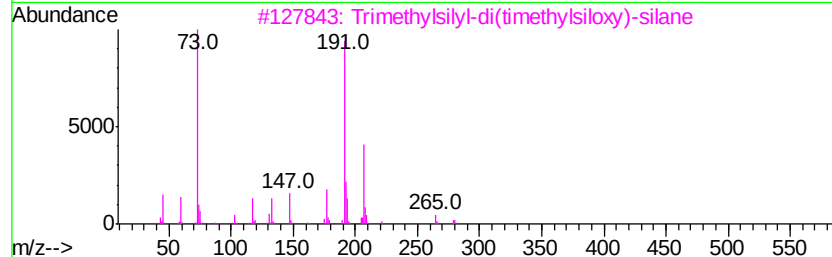
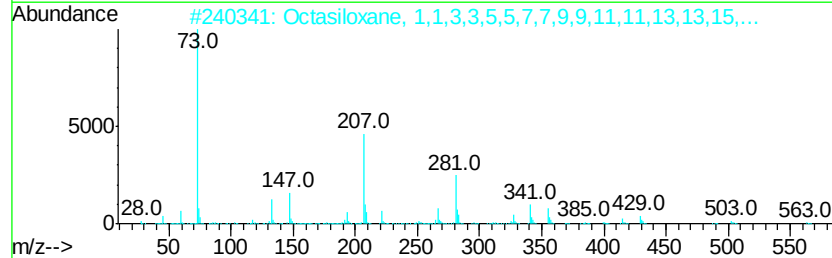
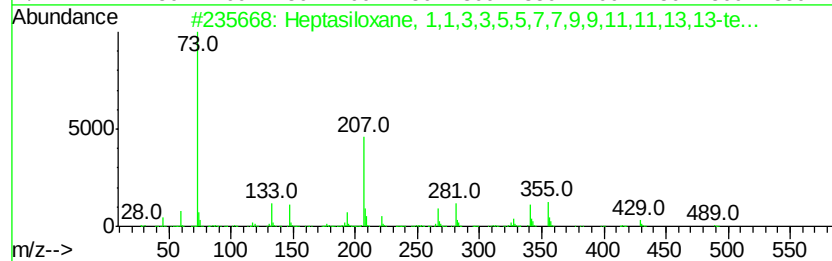
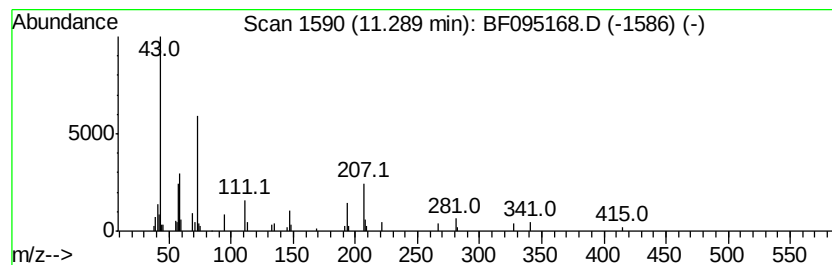
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Peak Number 5 unknown11.29 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.29	2.11 ng	97733	Acenaphthene-d10	12.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	38
2	Octasiloxane, 1,1,3,3,5,5,7,7,9...	578	C16H50O7Si8	019095-24-0	37
3	Trimethylsilyl-di(trimethylsiloxyl)...	280	C9H28O2Si4	139347-50-5	23
4	1-Monolinoleoylglycerol trimethyl...	498	C27H54O4Si2	054284-45-6	20
5	1,4-Dihydro-pyridine-3-carboxyli...	284	C16H16N2O3	1000259-17-8	18



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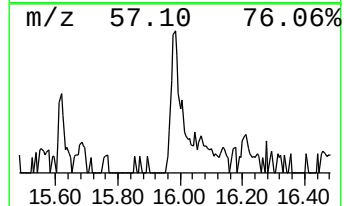
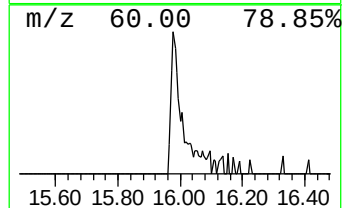
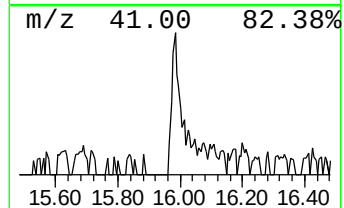
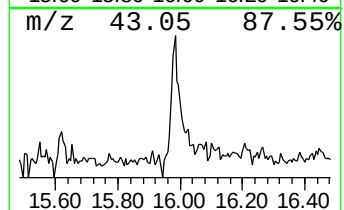
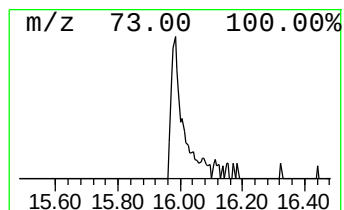
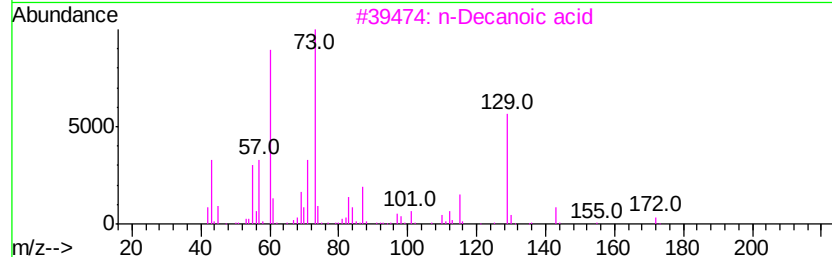
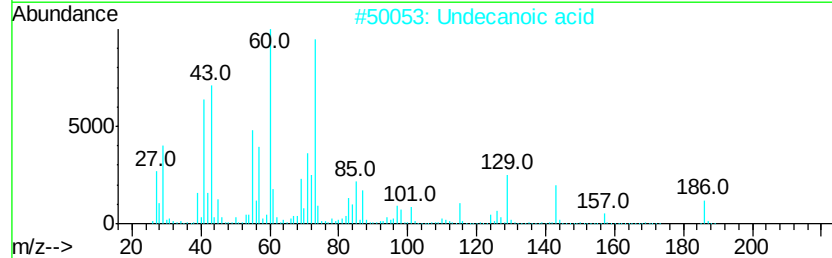
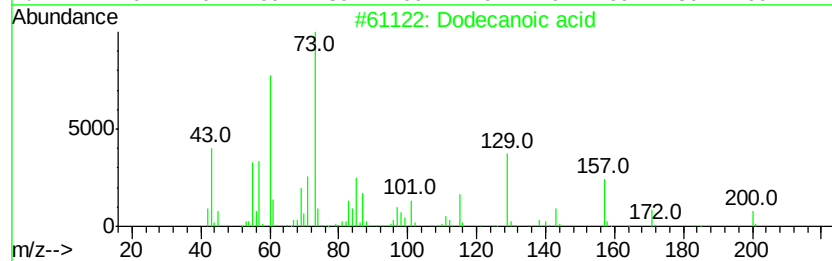
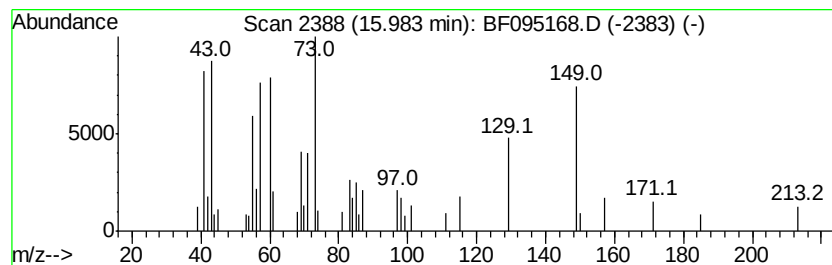
Instrument :
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ClientSampled :
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Dodecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.		
15.98	2.09 ng	79555	Phenanthrene-d10		15.02		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	52
2			Undecanoic acid	186	C11H22O2	000112-37-8	50
3			n-Decanoic acid	172	C10H20O2	000334-48-5	47
4			.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	38
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.15	15.6	ng	483752	1	7.78	621708	20.0
unknown7.44	7.44	98.9	ng	3075410	1	7.78	621708	20.0
Cyclohexasiloxane...	10.84	9.4	ng	395617	2	9.79	843345	20.0
unknown11.29	11.29	2.1	ng	97733	3	12.62	927284	20.0
Dodecanoic acid	15.98	2.1	ng	79555	4	15.02	761439	20.0