

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041621\
 Data File : BG048734.D
 Acq On : 16 Apr 2021 21:28
 Operator : CG/JU
 Sample : M2041-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S-2B

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_G\METHODS\8270-BG041421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048734.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.141	301	307	312	rBV	12927	17809	1.40%	0.277%
2	5.623	383	389	400	rVB	286466	456384	35.92%	7.095%
3	7.239	657	664	674	rBV	302977	532961	41.95%	8.285%
4	8.079	799	807	813	rVB2	88017	145453	11.45%	2.261%
5	9.248	999	1006	1014	rBV	195302	342160	26.93%	5.319%
6	10.905	1280	1288	1295	rBV	113378	204910	16.13%	3.186%
7	13.355	1697	1705	1711	rBV	499541	742234	58.42%	11.539%
8	14.177	1842	1845	1851	rVB3	10923	15766	1.24%	0.245%
9	14.736	1934	1940	1947	rVB2	185463	284350	22.38%	4.420%
10	16.228	2186	2194	2206	rBV2	435032	655832	51.62%	10.196%
11	17.491	2402	2409	2415	rBV	260385	386851	30.45%	6.014%
12	18.373	2554	2559	2563	rBV3	20365	31806	2.50%	0.494%
13	19.136	2684	2689	2693	rBV2	43247	56108	4.42%	0.872%
14	19.219	2698	2703	2708	rBV6	9732	14627	1.15%	0.227%
15	19.542	2753	2758	2765	rBV4	19340	28315	2.23%	0.440%
16	19.906	2817	2820	2826	rBV5	8461	13568	1.07%	0.211%
17	20.106	2848	2854	2859	rBV	992839	1270542	100.00%	19.752%
18	20.776	2964	2968	2973	rVB2	16909	27457	2.16%	0.427%
19	20.993	3001	3005	3010	rBV	54642	75157	5.92%	1.168%
20	21.375	3064	3070	3072	rBV6	10202	19569	1.54%	0.304%
21	21.410	3072	3076	3086	rVV4	63315	109333	8.61%	1.700%
22	21.498	3086	3091	3098	rVB2	13087	22212	1.75%	0.345%
23	21.792	3133	3141	3153	rBV2	261838	429840	33.83%	6.682%
24	21.980	3169	3173	3178	rVB5	11130	13929	1.10%	0.217%
25	22.991	3341	3345	3348	rBV5	8326	13155	1.04%	0.205%
26	23.320	3393	3401	3407	rVB10	9269	19131	1.51%	0.297%
27	23.519	3430	3435	3441	rBV7	13584	26676	2.10%	0.415%
28	25.135	3698	3710	3719	rBV2	139662	419842	33.04%	6.527%
29	26.334	3912	3914	3920	rVB6	7828	14086	1.11%	0.219%
30	31.551	4799	4802	4810	rVB9	17917	42500	3.35%	0.661%

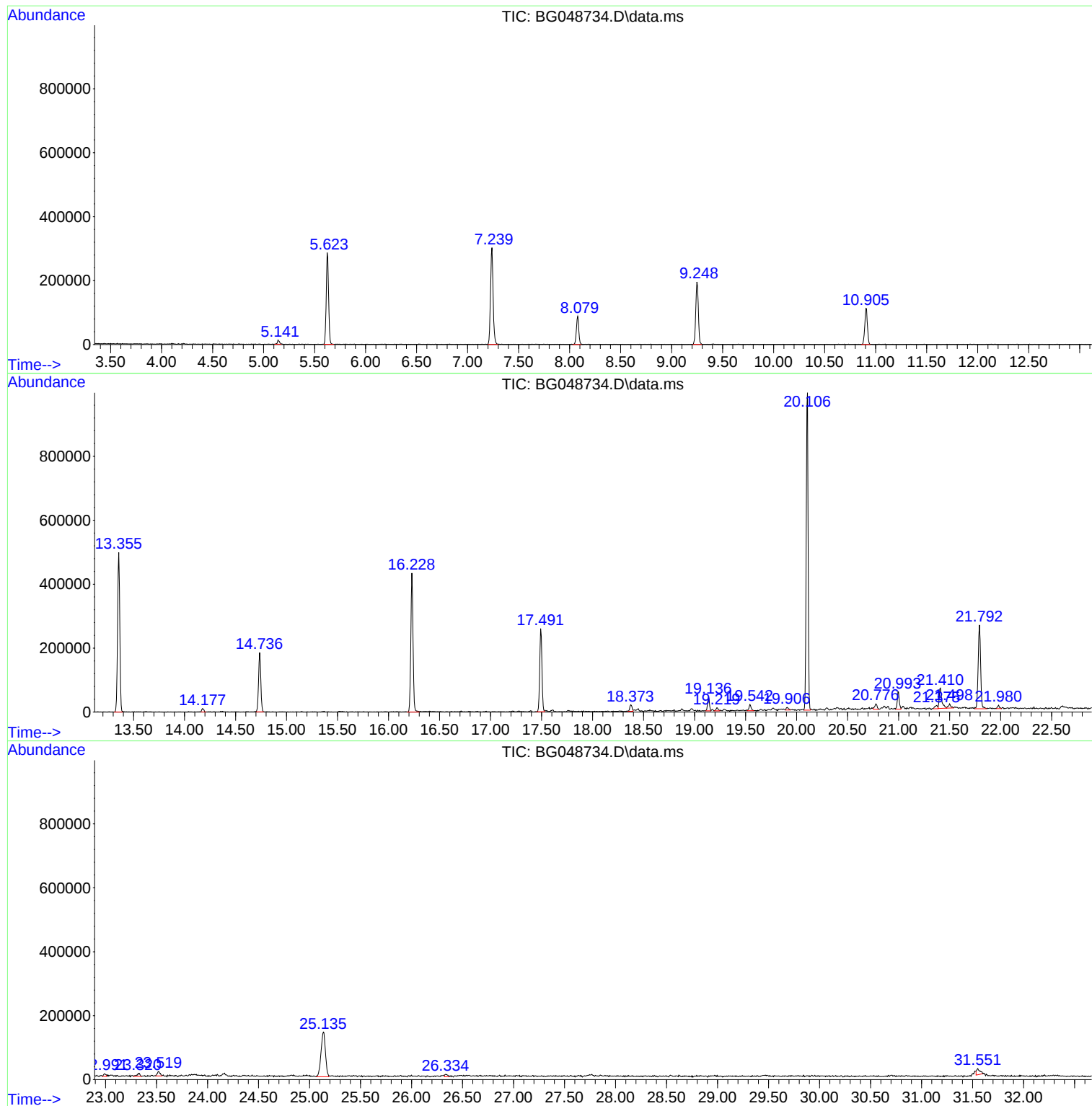
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S-2B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.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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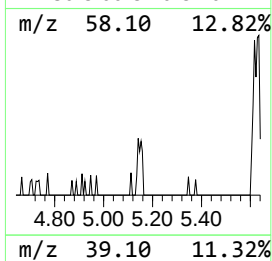
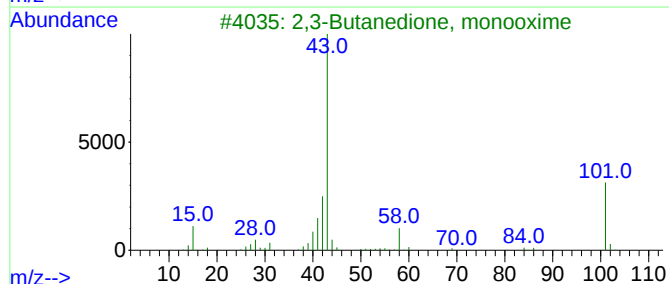
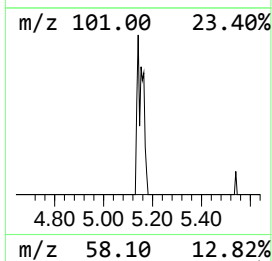
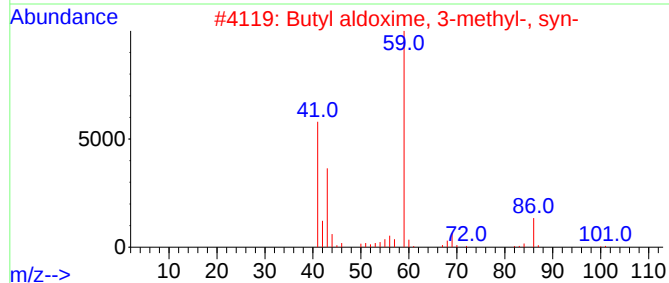
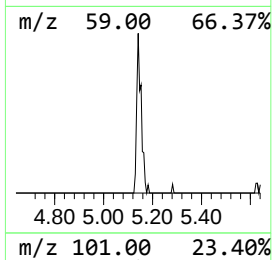
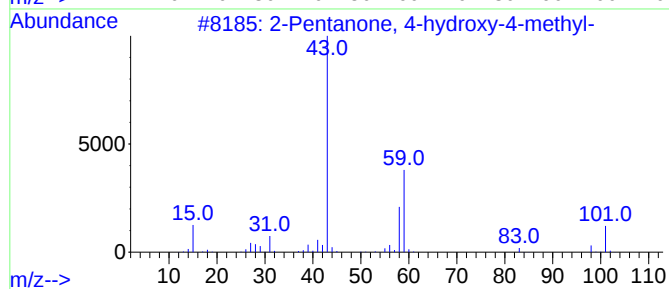
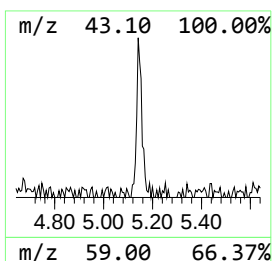
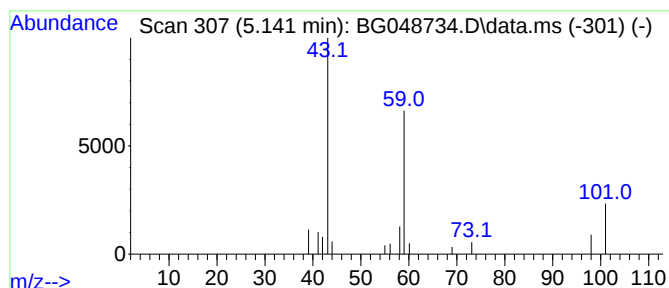
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.141	2.45 ng	17809	1,4-Dichlorobenzene-d4	8.079

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butanal, 3-methyl-, oxime	101	C5H11NO	000626-90-4	9



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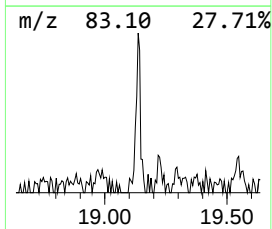
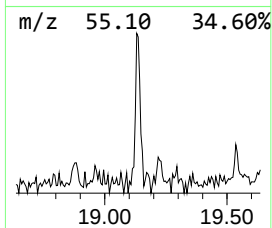
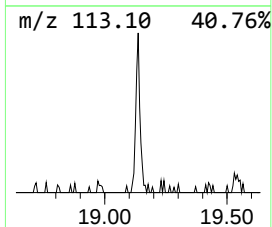
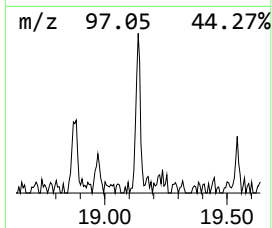
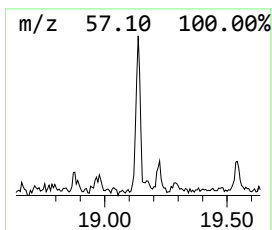
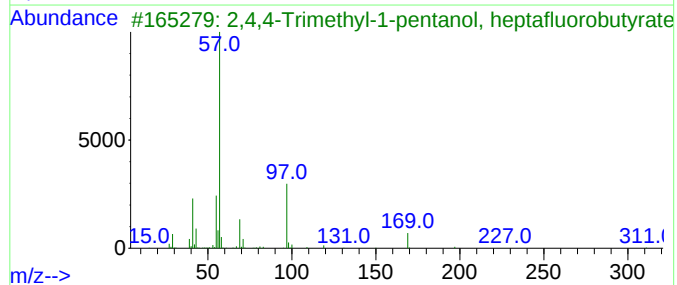
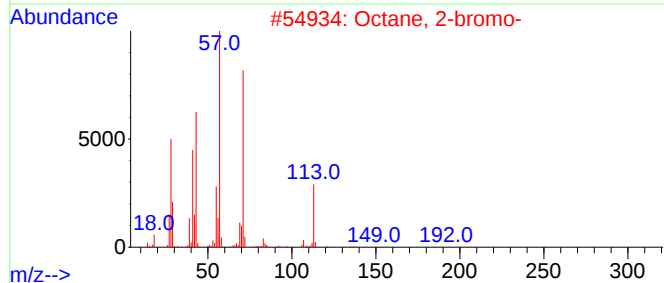
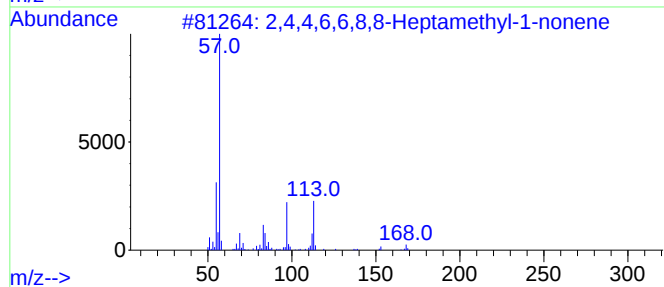
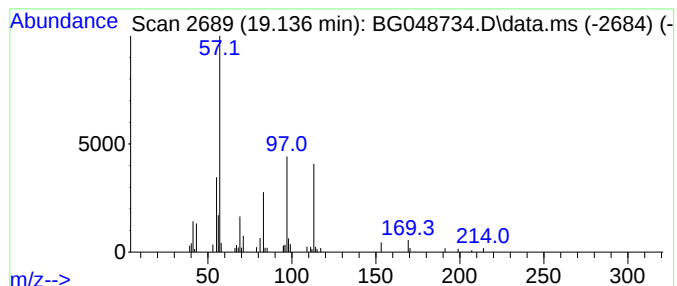
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Peak Number 2 unknown19.136 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.136	2.90 ng	56108	Phenanthrene-d10	17.491

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	45		
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35		
3	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	35		
4	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	27		
5	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	25		



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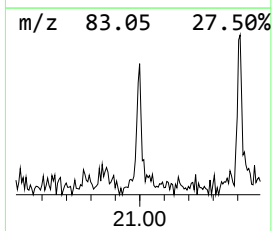
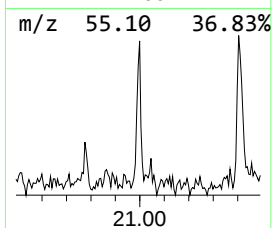
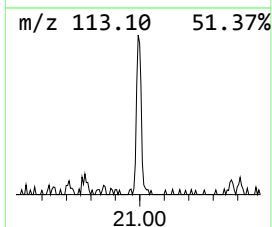
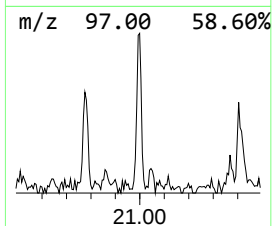
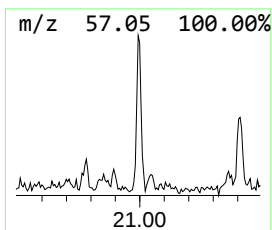
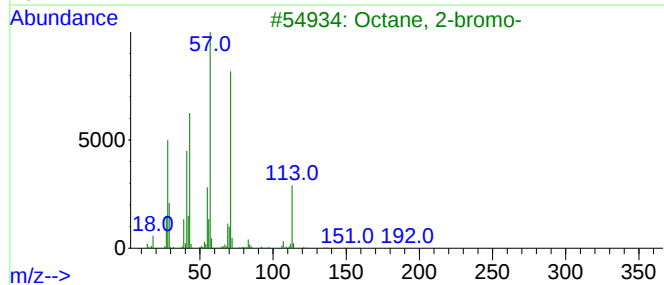
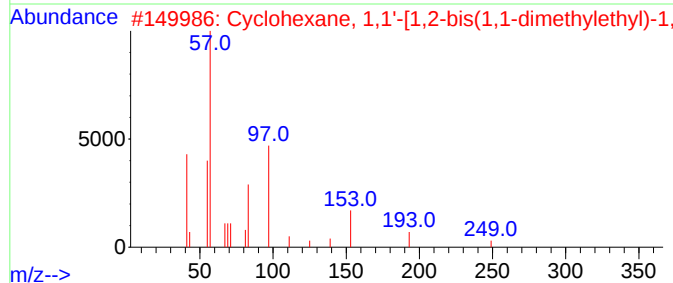
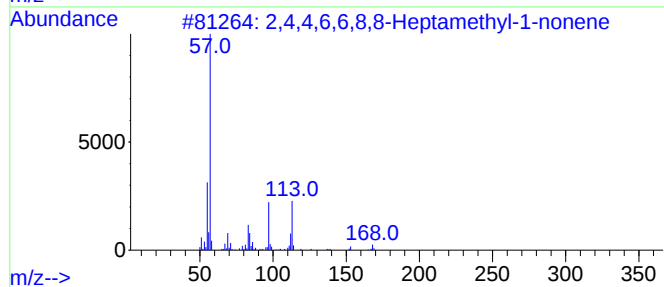
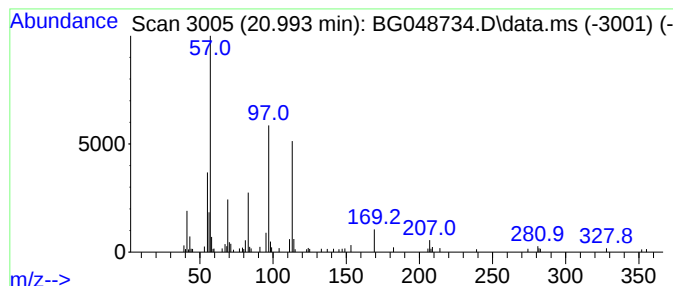
Instrument :
BNA_G
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Peak Number 3 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.993	3.50 ng	75157	Chrysene-d12	21.792	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	72
2	Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	37
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
4	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	16
5	Cyclohexane, 2,4-diisopropyl-1,1...	196	C14H28	1000149-60-5	16



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BNA_G
ClientSampled :
S-2B

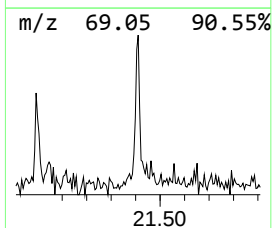
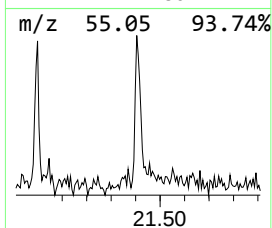
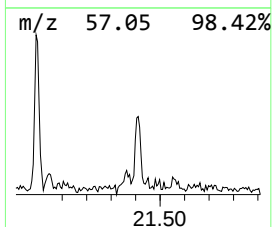
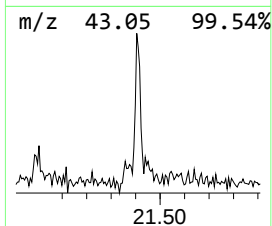
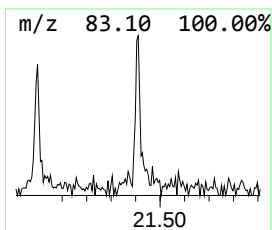
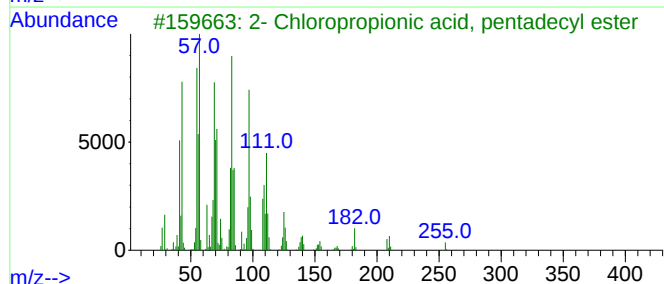
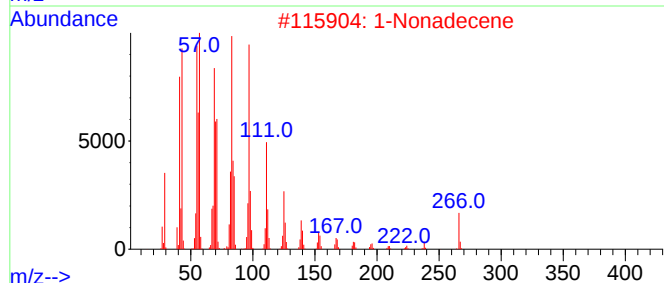
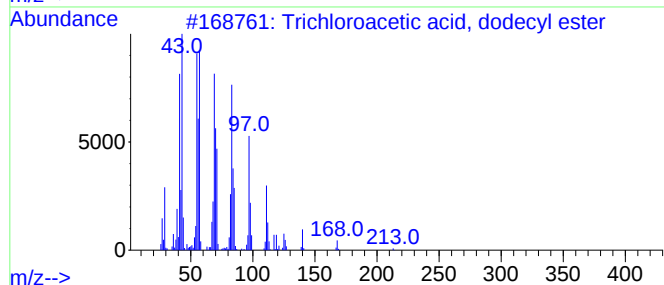
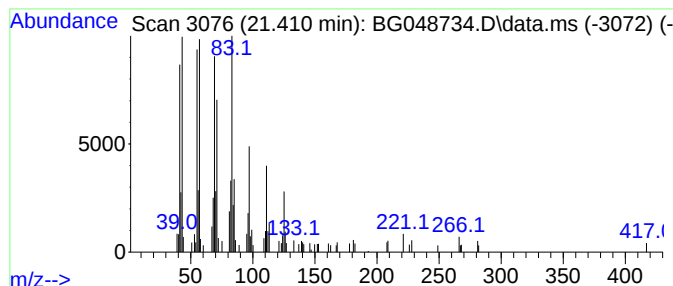
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Peak Number 4 Trichloroacetic acid, dodec... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.410	5.09 ng	109333	Chrysene-d12	21.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, dodecyl ester	330	C14H25Cl3O2	074339-50-7	80
2			1-Nonadecene	266	C19H38	018435-45-5	74
3			2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	64
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
5			Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	60



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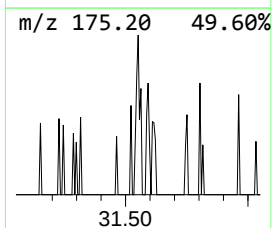
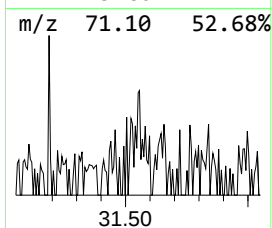
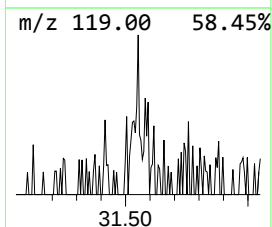
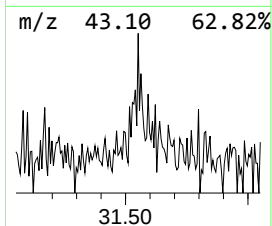
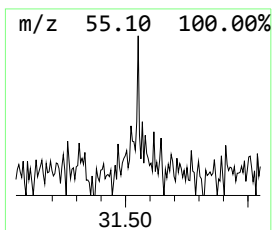
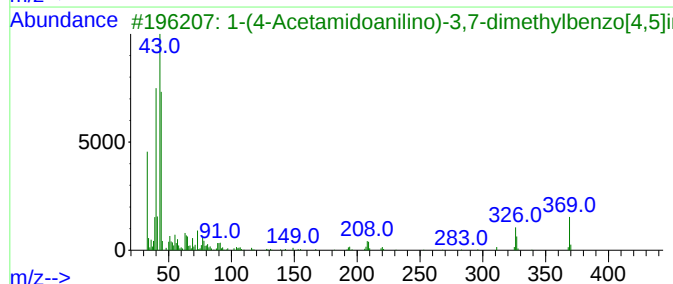
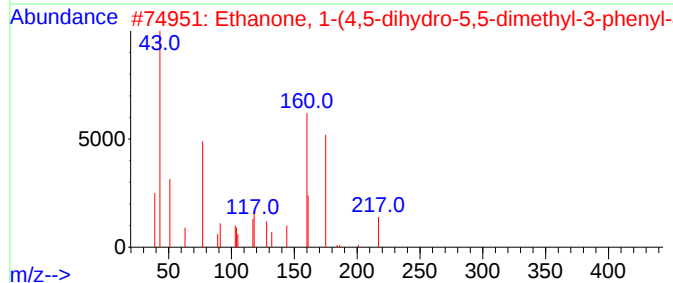
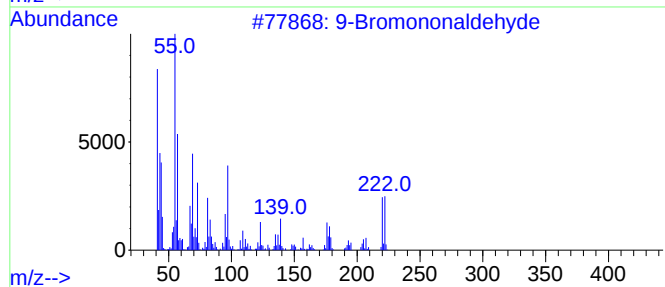
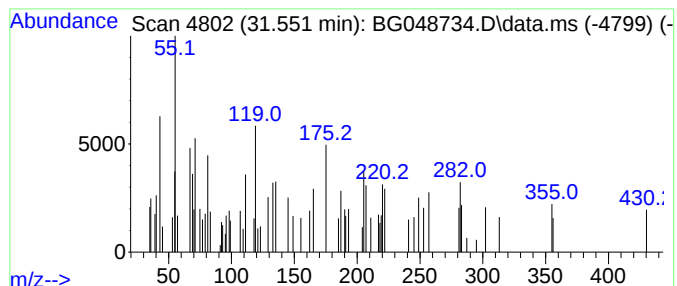
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Peak Number 5 unknown31.551 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.551	2.02 ng	42500	Perylene-d12	25.135

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Bromononaldehyde	220	C9H17BrO	124388-97-2	10
2			Ethanone, 1-(4,5-dihydro-5,5-dimethyl-3-phenyl-)	217	C13H15NO2	042812-87-3	9
3			1-(4-Acetamidoanilino)-3,7-dimethylbenzo[4,5-j]keto[1,2-b:4,5-f']oxazole	369	C22H19N5O	299200-97-8	9
4			L-Histidine, N-[(2,4-dichlorophenyl)amino]-	357	C14H13Cl2N3O4	050649-03-1	7
5			3.alpha.,4.alpha.-Epoxymuroalan-9-one	236	C15H24O2	1000140-33-2	7



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.141	2.5	ng	17809	1	8.079	145453	20.0
unknown19.136	19.136	2.9	ng	56108	4	17.491	386851	20.0
2,4,4,6,6,8,8-H...	20.993	3.5	ng	75157	5	21.792	429840	20.0
Trichloroacetic...	21.410	5.1	ng	109333	5	21.792	429840	20.0
unknown31.551	31.551	2.0	ng	42500	6	25.135	419842	20.0