

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011221\
 Data File : BP004519.D
 Acq On : 12 Jan 2021 23:19
 Operator : CG/JU
 Sample : M1078-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 NB-07-011121

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_P\METHODS\8270E-BP011221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004519.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.399	369	376	394	rBV	2389672	3657267	41.19%	7.409%
2	6.981	637	645	662	rBV	2226312	3747178	42.20%	7.591%
3	7.810	779	786	794	rBV	693143	1128137	12.70%	2.285%
4	8.969	975	983	999	rBV	1398203	2374829	26.74%	4.811%
5	10.604	1253	1261	1275	rBV	905806	1585458	17.86%	3.212%
6	13.075	1673	1681	1696	rBV	3788133	5762897	64.90%	11.675%
7	13.916	1817	1824	1833	rBV	78180	132559	1.49%	0.269%
8	14.463	1906	1917	1925	rBV	1462884	2208356	24.87%	4.474%
9	15.957	2164	2171	2189	rBV	3241462	4893715	55.11%	9.914%
10	17.222	2380	2386	2391	rBV	1822713	2672600	30.10%	5.414%
11	18.598	2615	2620	2631	rBV	57184	124436	1.40%	0.252%
12	18.851	2658	2663	2668	rBV	463767	551016	6.21%	1.116%
13	18.939	2674	2678	2682	rBV	126714	156633	1.76%	0.317%
14	19.239	2724	2729	2734	rBV	288256	411430	4.63%	0.834%
15	19.468	2764	2768	2772	rBV	123069	147599	1.66%	0.299%
16	19.592	2785	2789	2797	rVB	259562	387825	4.37%	0.786%
17	19.786	2816	2822	2835	rBV	7221881	8879580	100.00%	17.989%
18	20.451	2932	2935	2942	rVB	129555	176357	1.99%	0.357%
19	20.657	2966	2970	2975	rBV	508359	596371	6.72%	1.208%
20	20.704	2975	2978	2985	rVB	113896	135298	1.52%	0.274%
21	20.986	3021	3026	3029	rBV2	133322	250984	2.83%	0.508%
22	21.033	3029	3034	3040	rVV3	464234	959307	10.80%	1.943%
23	21.092	3040	3044	3050	rVB	565643	752724	8.48%	1.525%
24	21.315	3076	3082	3086	rBV	2796377	3723541	41.93%	7.543%
25	21.351	3086	3088	3097	rVB	165473	189269	2.13%	0.383%
26	22.951	3357	3360	3366	rBV	112663	208636	2.35%	0.423%
27	23.668	3475	3482	3490	rBV2	1819842	3547698	39.95%	7.187%

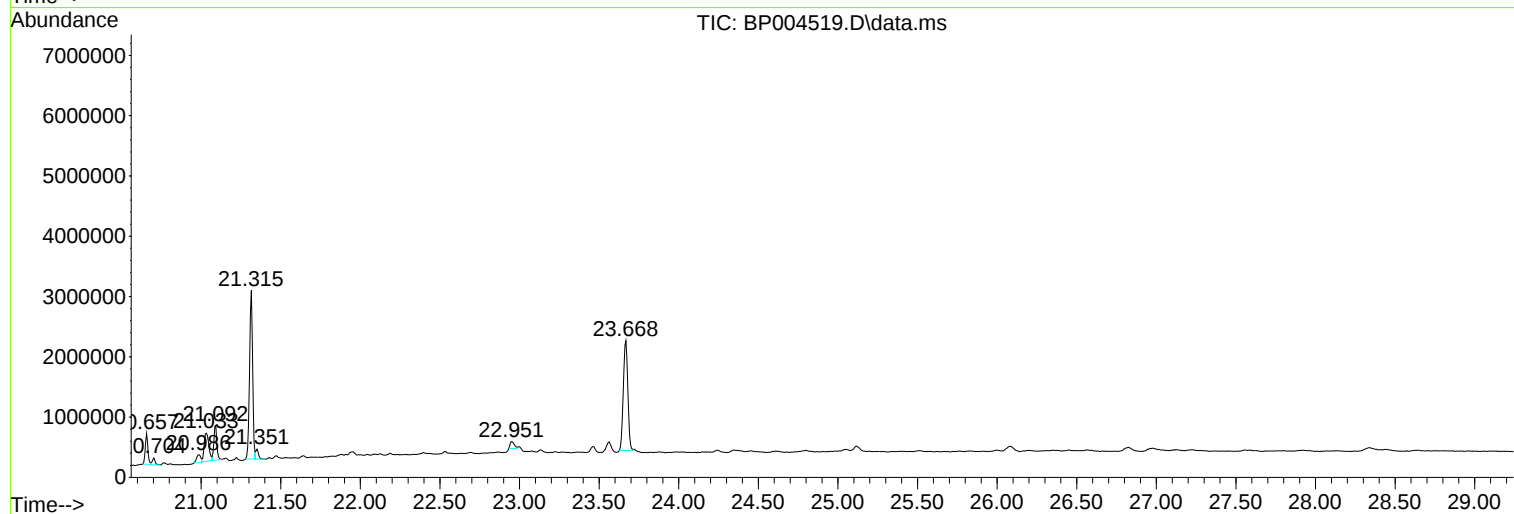
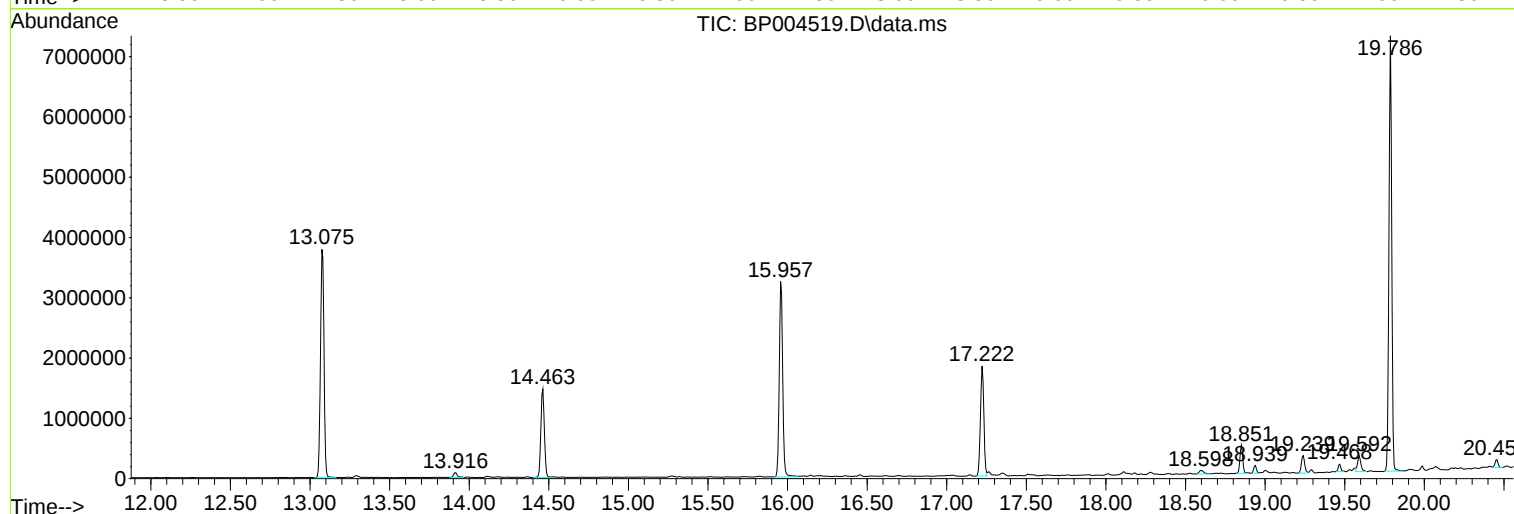
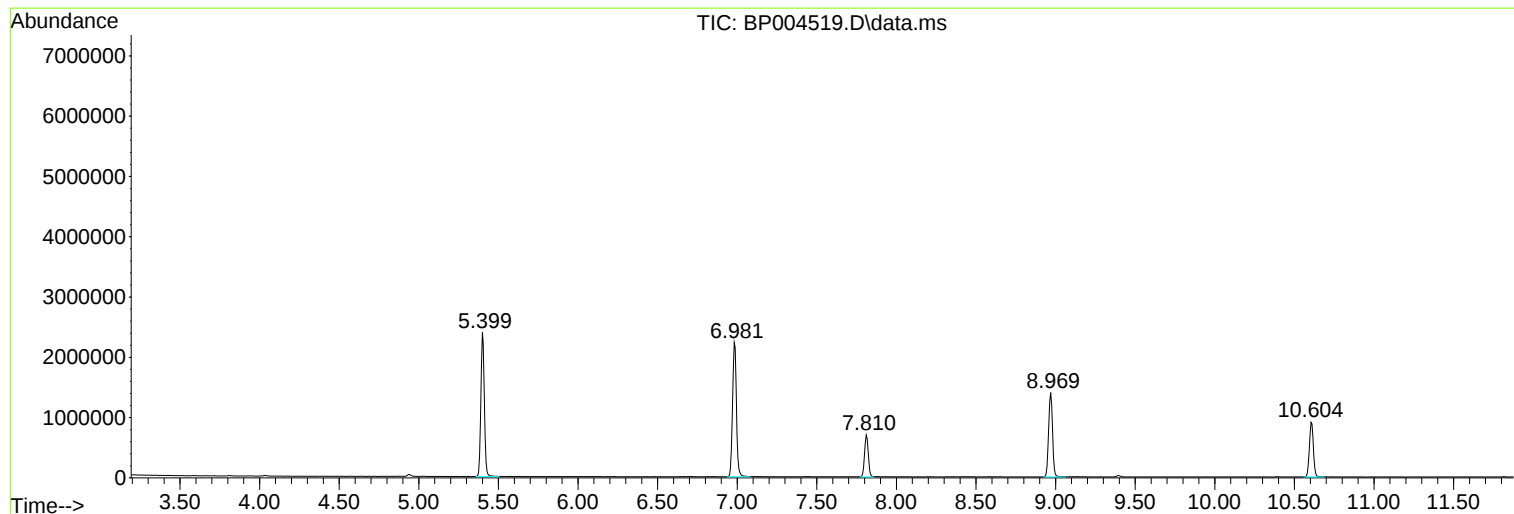
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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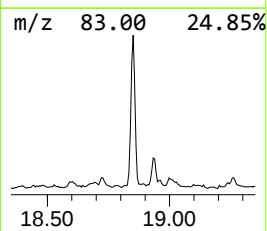
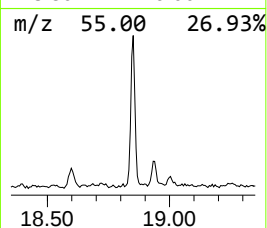
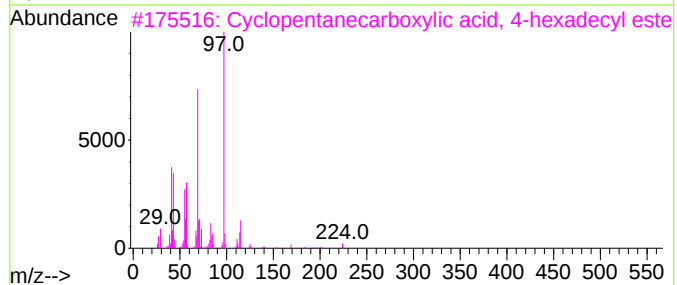
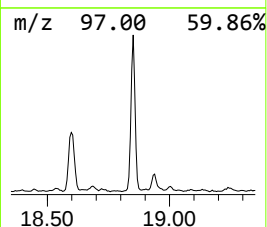
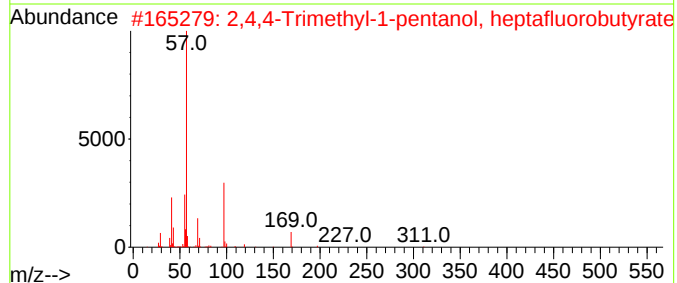
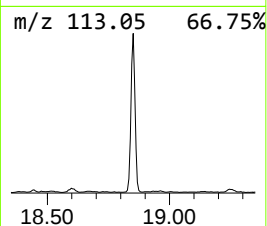
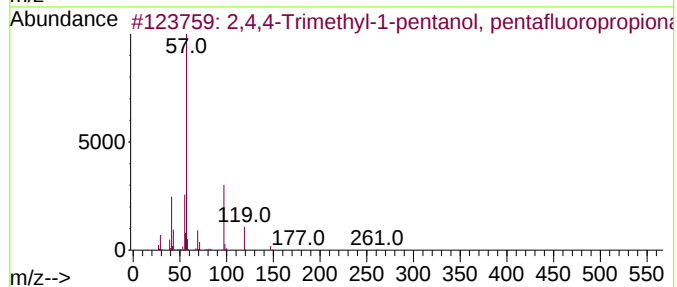
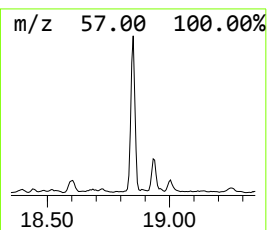
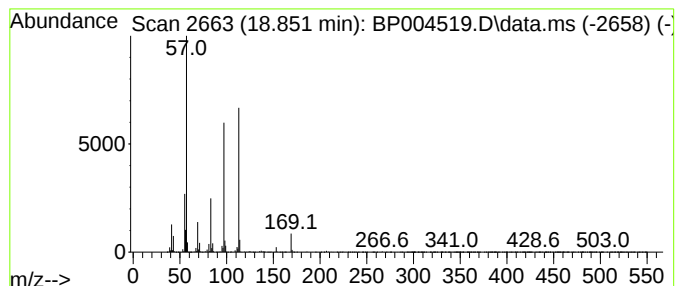
Instrument :
BNA_P
ClientSampleId :
NB-07-011121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown18.851 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.851	4.12 ng	551016	Phenanthrene-d10	17.221	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	38
2	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	38
3	Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	35
4	Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	35
5	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35



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ClientSampleId :
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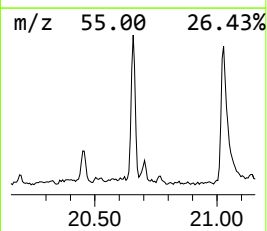
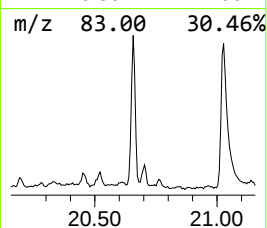
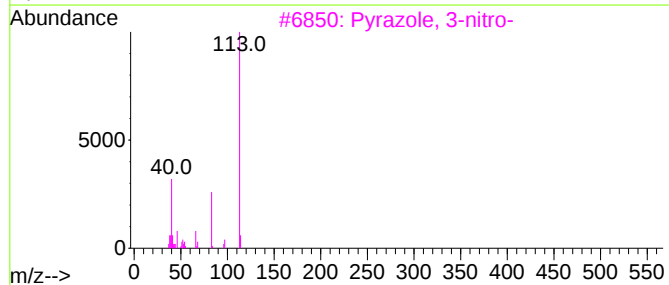
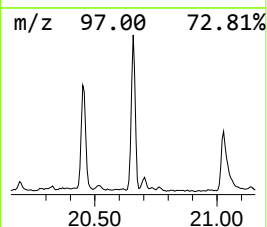
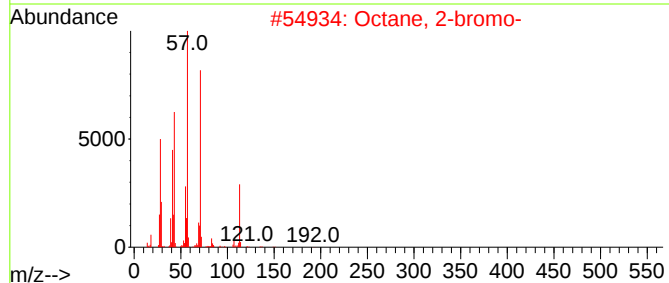
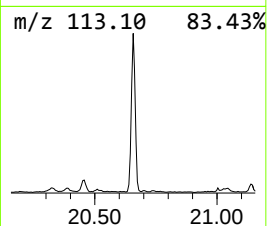
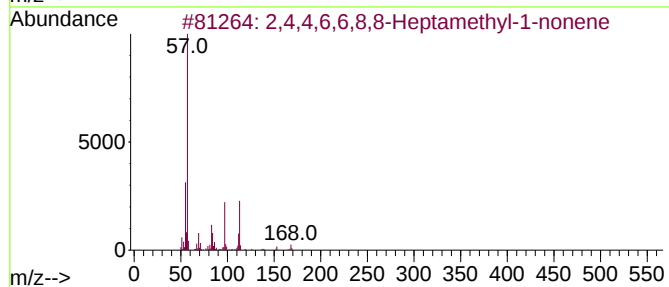
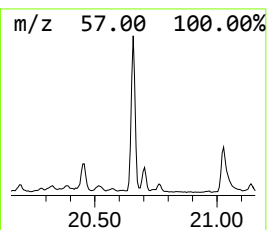
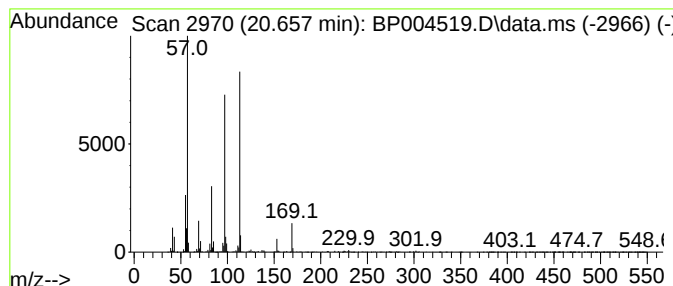
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Peak Number 3 unknown20.657 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.657	3.20 ng	596371	Chrysene-d12	21.315

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	47		
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	43		
3	Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	43		
4	Acetamide, 2-(4-methyl-1-piperaz...	267	C13H18ClN3O	296245-55-1	38		
5	.beta.-D-Fructopyranose, 2,3:4,5...	368	C17H30B207	1000156-76-8	37		



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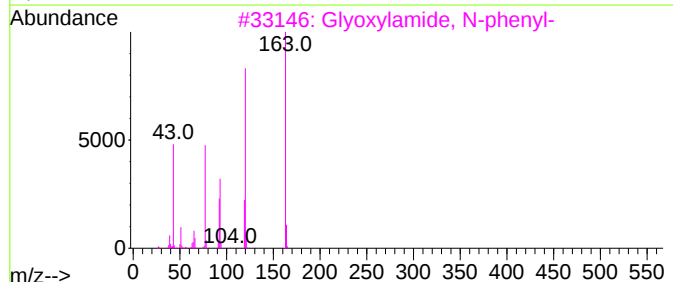
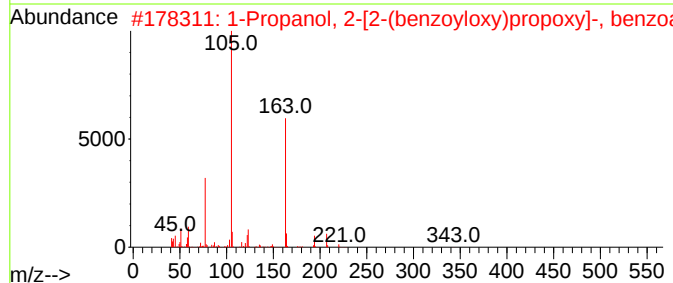
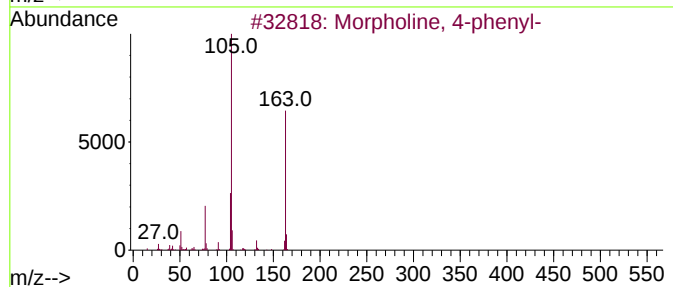
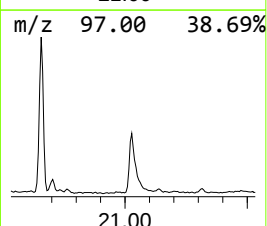
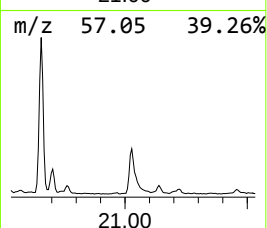
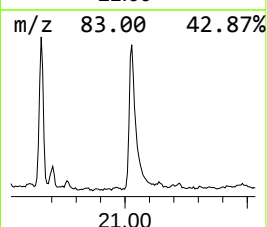
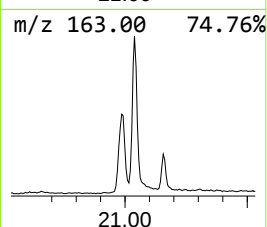
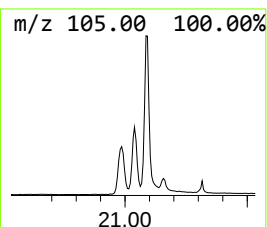
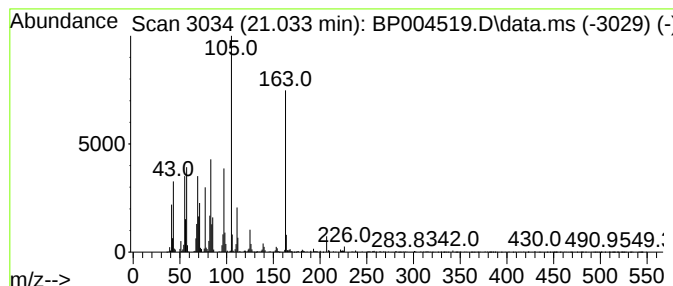
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Peak Number 4 unknown21.033 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.033	5.15 ng	959307	Chrysene-d12	21.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	35
2			1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	25
3			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	22
4			1,3-Dioxolane, 2,4-dimethyl-2-ph...	178	C11H14O2	004359-30-2	17
5			5-Fluoro-8-quinolinol	163	C9H6FNO	000387-97-3	14



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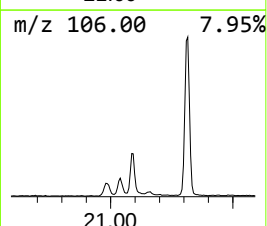
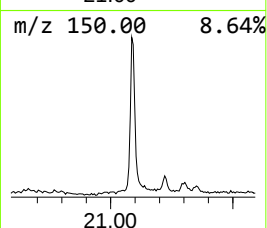
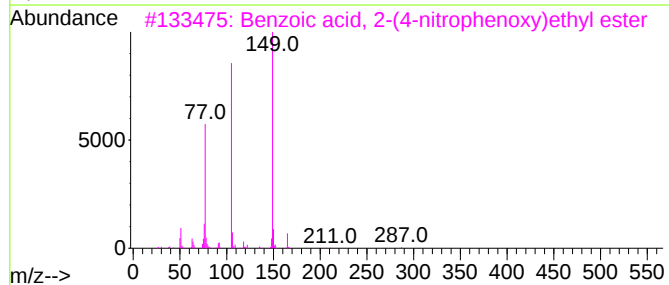
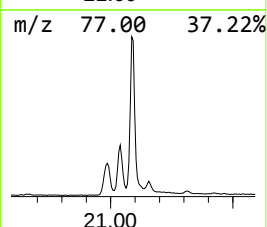
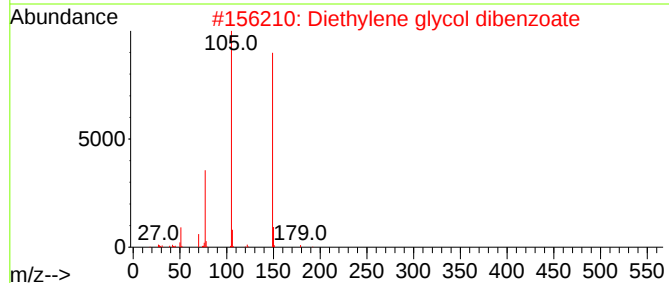
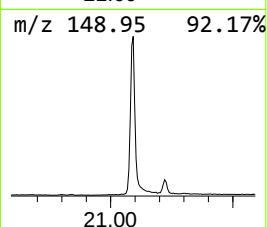
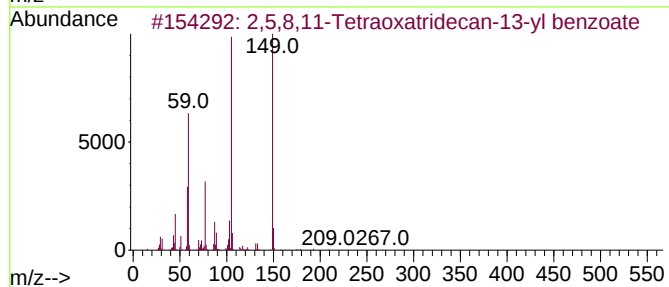
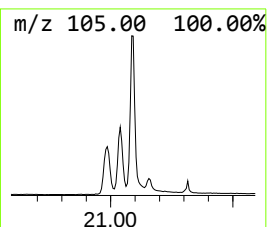
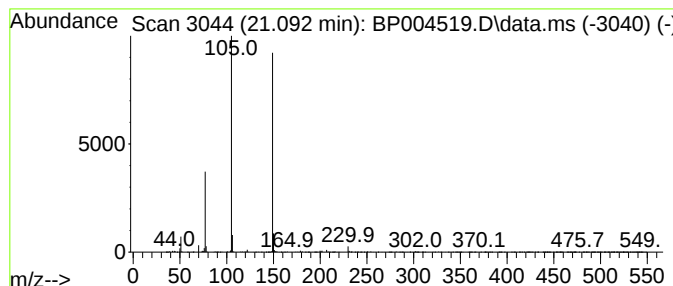
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Peak Number 5 2,5,8,11-Tetraoxatridecan-1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	4.04 ng	752724	Chrysene-d12	21.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	78		
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78		
3	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78		
4	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64		
5	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	64		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown20.657	20.657	3.2	ng	596371	5	21.315	3723540	20.0
unknown21.033	21.033	5.2	ng	959307	5	21.315	3723540	20.0
2,5,8,11-Tetrao...	21.092	4.0	ng	752724	5	21.315	3723540	20.0