

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010721\
 Data File : BP004485.D
 Acq On : 07 Jan 2021 18:04
 Operator : CG/JU
 Sample : M1019-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 20410

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-BP121120.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004485.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.940	294	298	311	rVB	291969	440580	3.44%	0.597%
2	5.405	371	377	388	rVB	4056000	5970604	46.59%	8.084%
3	6.987	638	646	660	rBV	3969076	6736001	52.56%	9.120%
4	7.816	780	787	794	rBV	1169257	1894899	14.79%	2.566%
5	8.969	975	983	994	rBV	2604513	4416601	34.47%	5.980%
6	10.610	1254	1262	1270	rBV	1537456	2704348	21.10%	3.661%
7	13.081	1673	1682	1694	rBV	6848246	10220452	79.76%	13.838%
8	13.916	1818	1824	1828	rBV	165202	238152	1.86%	0.322%
9	14.463	1907	1917	1925	rBV	2387843	3549992	27.70%	4.806%
10	15.957	2164	2171	2189	rBV	4875948	7376839	57.57%	9.988%
11	17.228	2378	2387	2392	rBV	2612973	3972875	31.00%	5.379%
12	17.516	2431	2436	2447	rBV2	78970	160835	1.26%	0.218%
13	18.116	2533	2538	2545	rBV3	119354	202271	1.58%	0.274%
14	18.186	2546	2550	2554	rVB	128993	154585	1.21%	0.209%
15	18.604	2617	2621	2631	rVB	88497	179705	1.40%	0.243%
16	18.857	2659	2664	2669	rBV	707647	883001	6.89%	1.196%
17	18.939	2674	2678	2682	rVV	209502	253061	1.97%	0.343%
18	19.239	2725	2729	2737	rVB	275034	392995	3.07%	0.532%
19	19.475	2765	2769	2773	rBV	215676	249733	1.95%	0.338%
20	19.592	2786	2789	2798	rVB	211011	323753	2.53%	0.438%
21	19.792	2817	2823	2828	rBV	10303761	12814621	100.00%	17.350%
22	19.992	2853	2857	2862	rBV	142465	173697	1.36%	0.235%
23	20.463	2932	2937	2943	rVB	294859	373207	2.91%	0.505%
24	20.527	2943	2948	2953	rBV4	74944	144832	1.13%	0.196%
25	20.663	2967	2971	2975	rBV	1465743	1675446	13.07%	2.268%
26	20.710	2975	2979	2983	rVV	346227	412535	3.22%	0.559%
27	20.769	2986	2989	2999	rVB2	115839	187442	1.46%	0.254%
28	21.033	3030	3034	3042	rBV3	190520	388487	3.03%	0.526%
29	21.145	3050	3053	3060	rVB	138677	176358	1.38%	0.239%
30	21.321	3077	3083	3087	rBV	2722061	3683463	28.74%	4.987%
31	22.545	3287	3291	3296	rVB	94449	138472	1.08%	0.187%
32	22.951	3356	3360	3367	rBV3	116762	262179	2.05%	0.355%
33	23.674	3475	3483	3499	rVB2	1491209	3107189	24.25%	4.207%

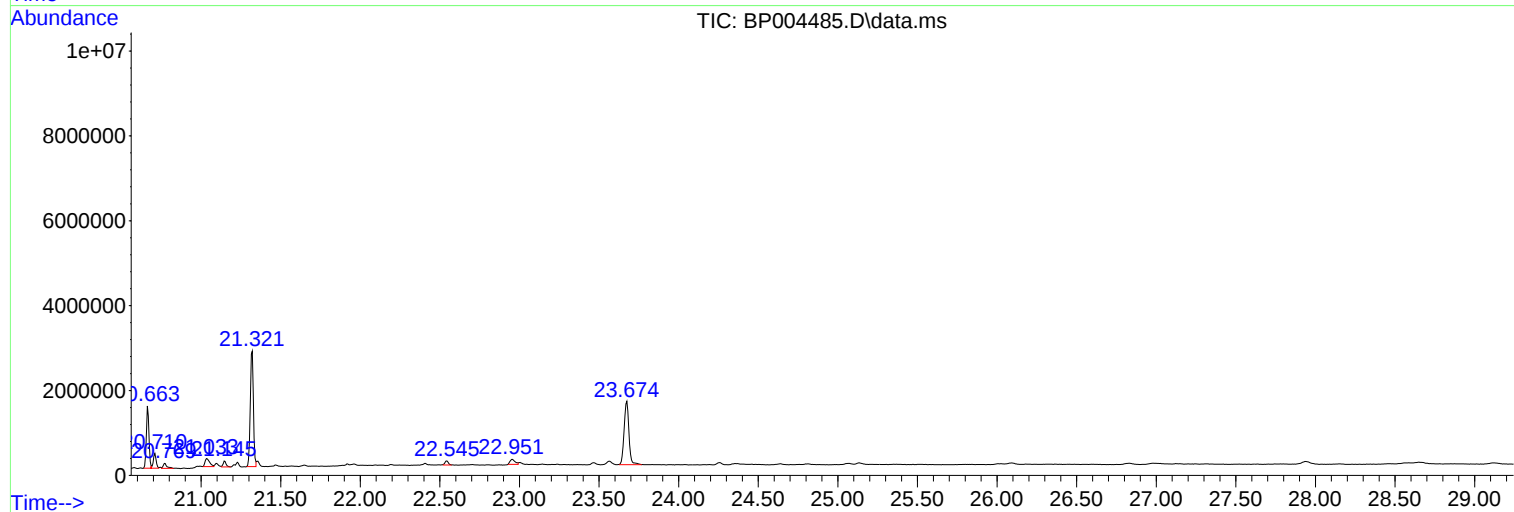
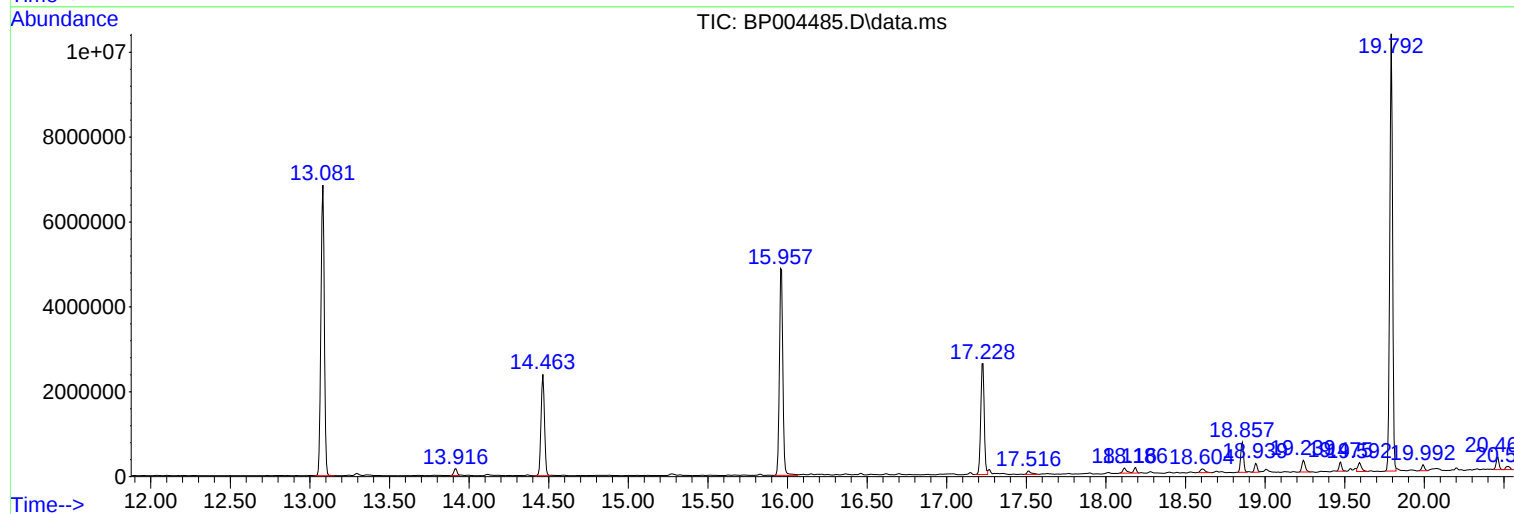
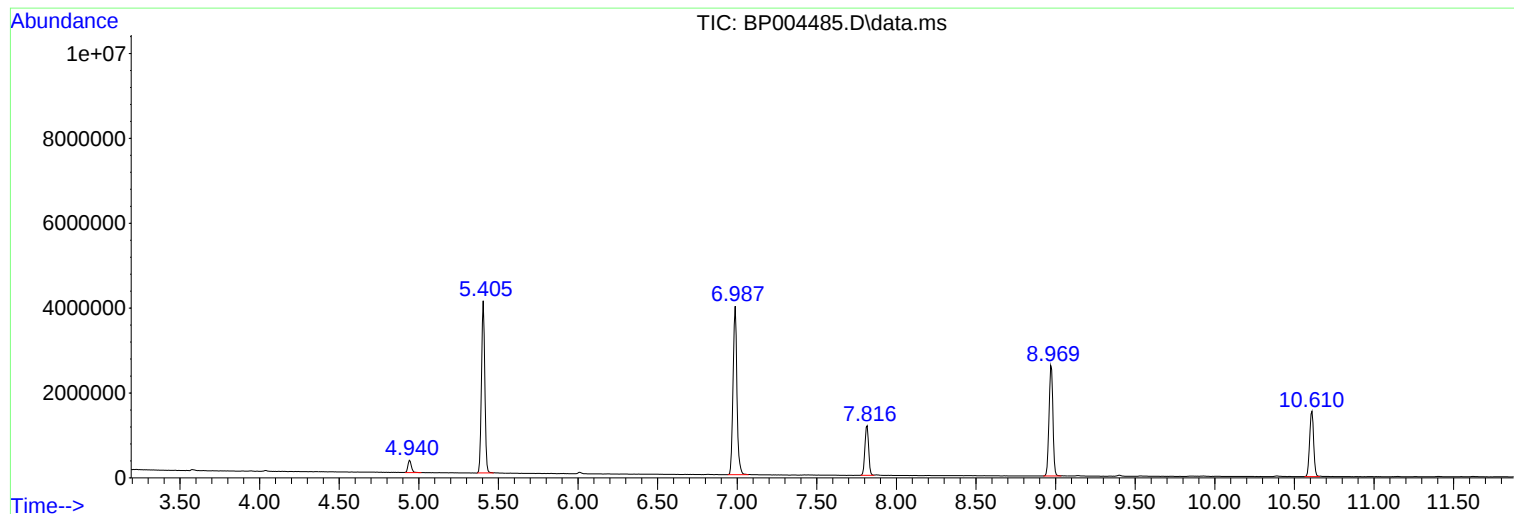
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP121120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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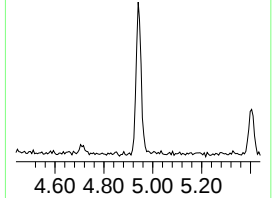
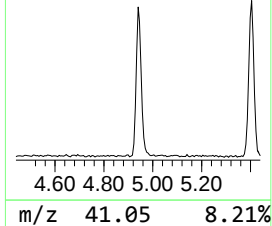
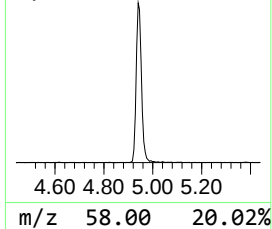
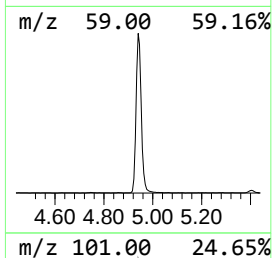
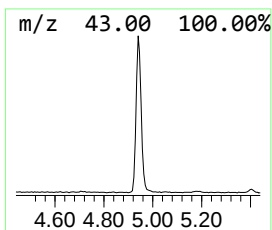
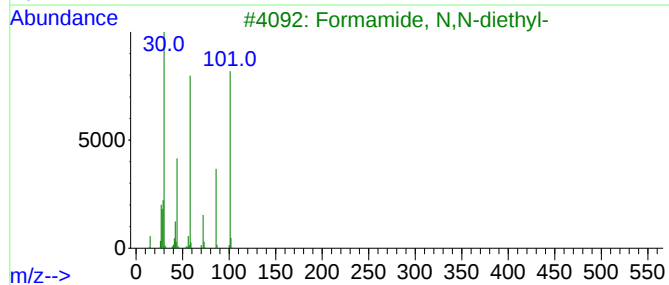
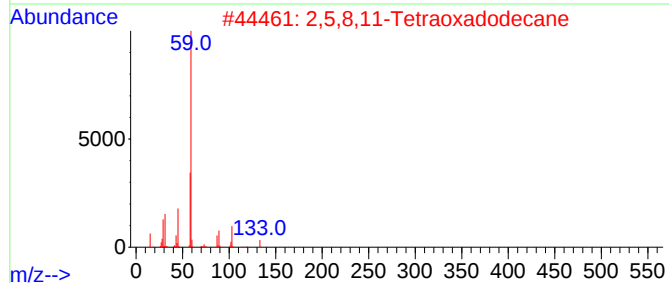
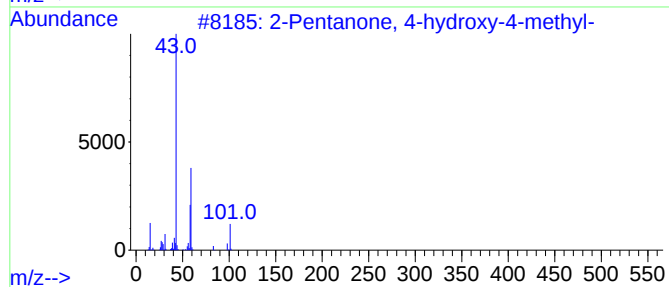
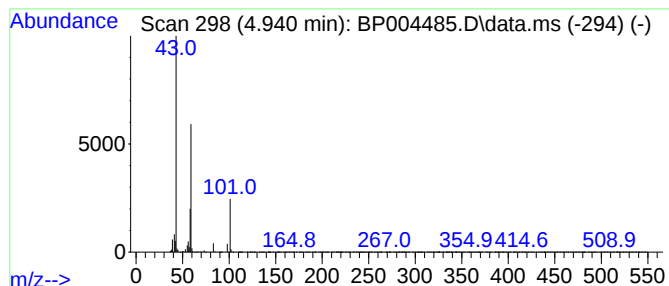
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.940	4.65 ng	440580	1,4-Dichlorobenzene-d4	7.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42		
2	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	23		
3	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	16		
4	Acetone	58	C3H6O	000067-64-1	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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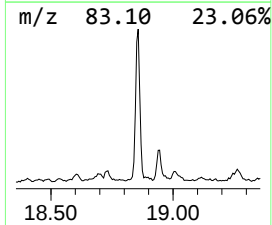
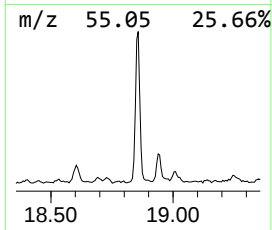
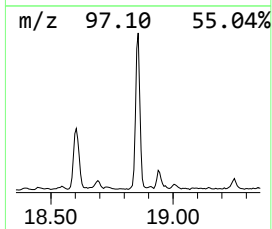
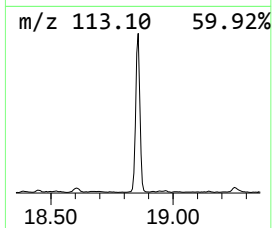
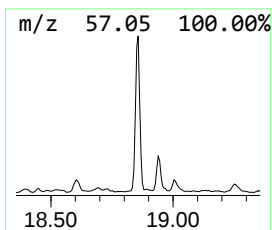
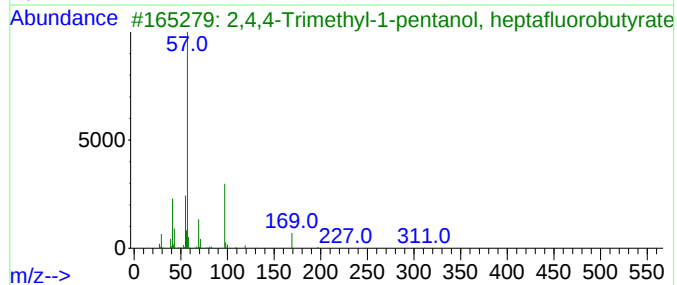
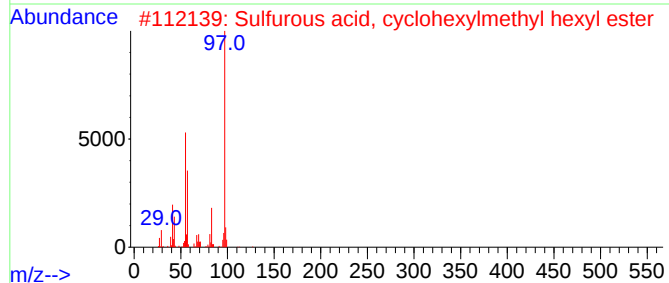
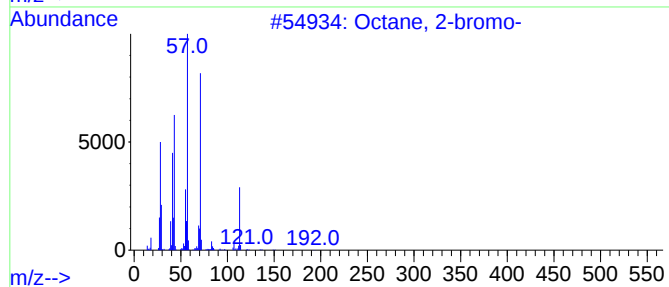
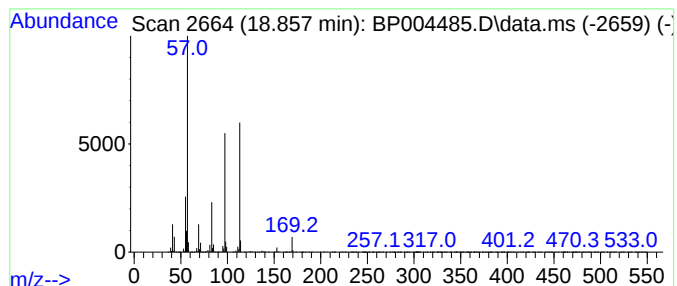
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown18.857 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.857	4.45 ng	883001	Phenanthrene-d10	17.228

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-bromo-		192	C8H17Br		000557-35-7	38
2	Sulfurous acid, cyclohexylmethyl...		262	C13H26O3S		1000309-21-6	38
3	2,4,4-Trimethyl-1-pentanol, hept...		326	C12H17F7O2		1000365-01-4	37
4	2,4,4-Trimethyl-1-pentanol, pent...		276	C11H17F5O2		1000365-51-0	32
5	Sulfurous acid, cyclohexylmethyl...		304	C16H32O3S		1000309-21-8	32



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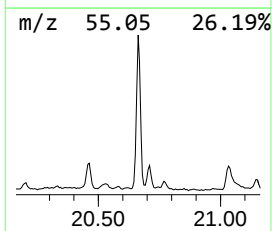
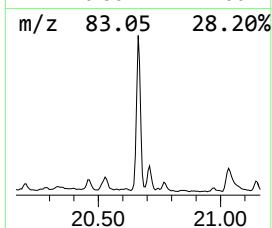
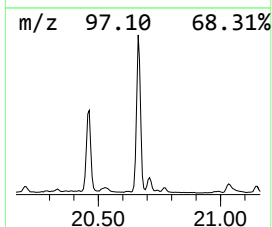
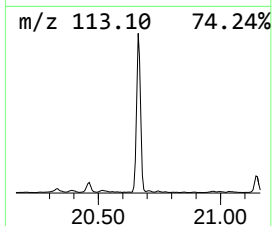
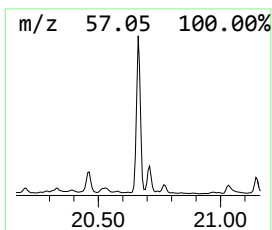
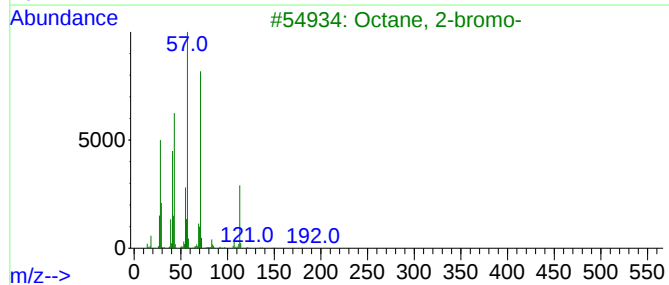
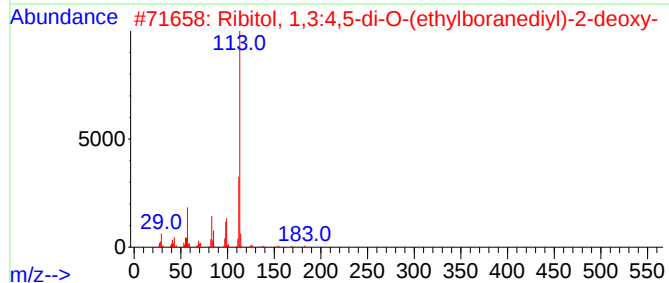
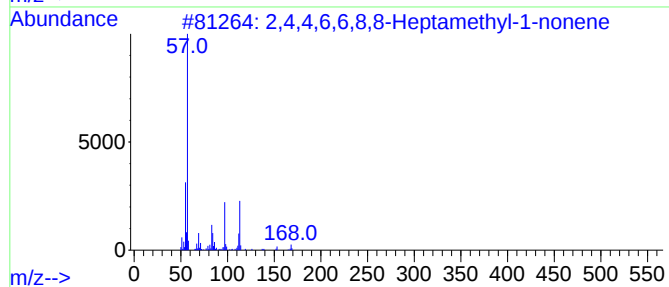
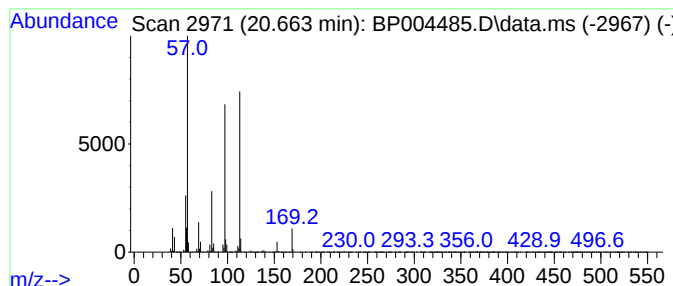
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.663	9.10 ng	1675450	Chrysene-d12	21.322

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	78		
2	Ribitol, 1,3:4,5-di-O-(ethylbora...	212	C9H18B2O4	1000149-52-8	37		
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	37		
4	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	37		
5	(E)-3-(Dimethylamino)-2-pentene	113	C7H15N	032317-47-8	35		



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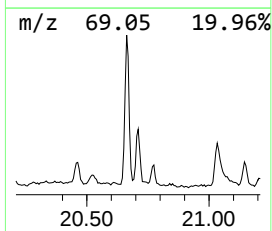
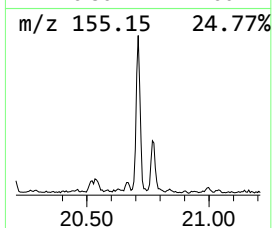
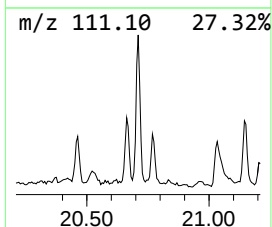
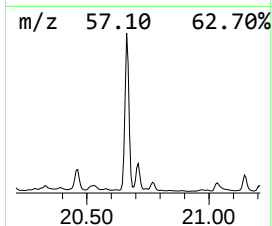
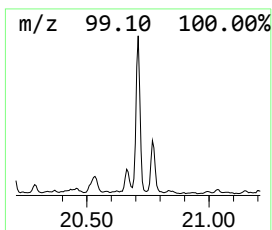
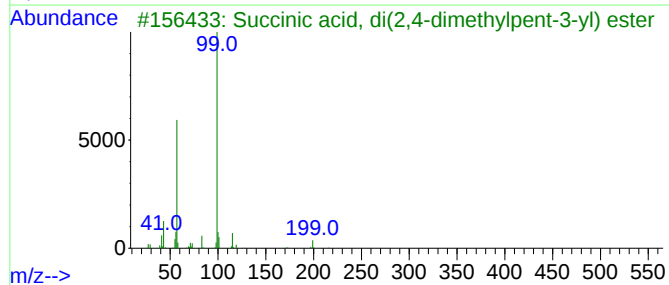
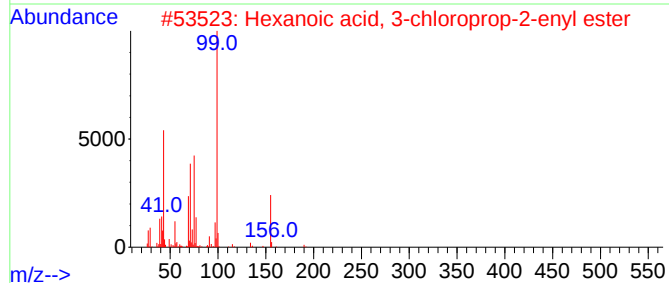
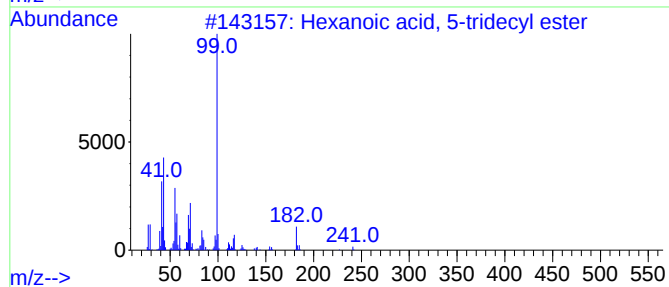
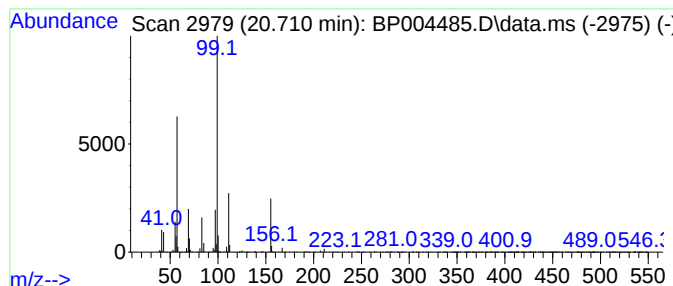
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Peak Number 4 unknown20.710 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.710	2.24 ng	412535	Chrysene-d12	21.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 5-tridecyl ester	298	C19H38O2	1000279-29-4	42
2			Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	42
3			Succinic acid, di(2,4-dimethylpe...	314	C18H34O4	1000349-36-7	38
4			1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	33
5			Tributyl phosphate	266	C12H27O4P	000126-73-8	33



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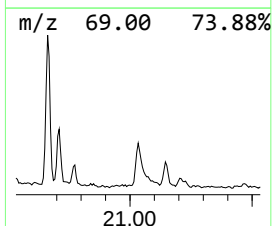
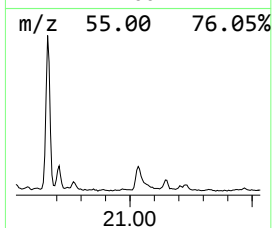
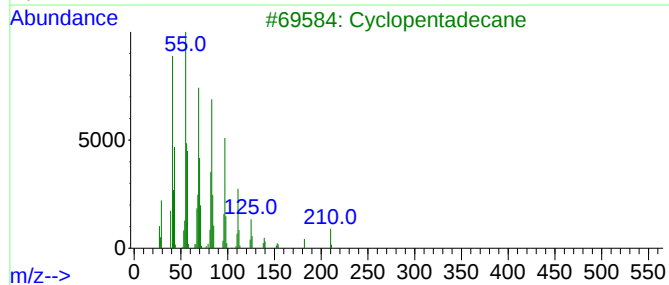
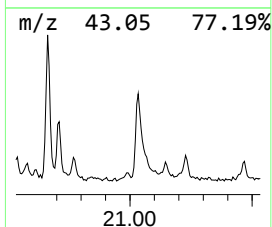
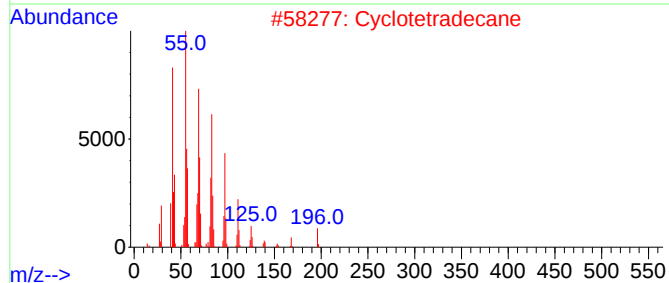
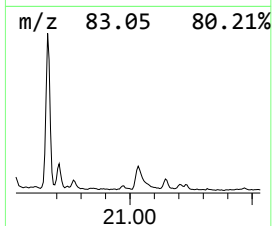
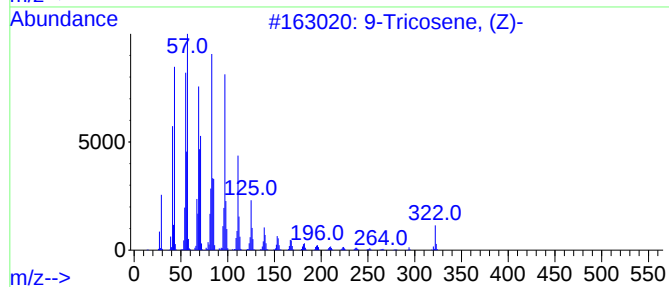
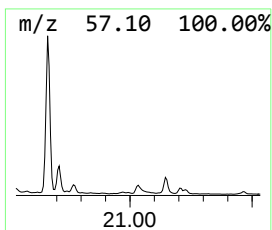
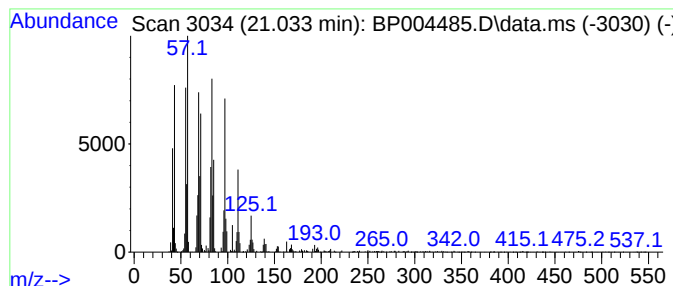
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Peak Number 5 9-Tricosene, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.033	2.11 ng	388487	Chrysene-d12	21.322

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	99	
2	Cyclotetradecane	196	C14H28	000295-17-0	97	
3	Cyclopentadecane	210	C15H30	000295-48-7	94	
4	1-Heptacosanol	396	C27H56O	002004-39-9	94	
5	1-Heneicosanol	312	C21H44O	015594-90-8	93	



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ClientSampleId :
20410

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP121120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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-...	4.940	4.7	ng	440580	1	7.816	1894900	20.0
unknown18.857	18.857	4.5	ng	883001	4	17.228	3972880	20.0
2,4,4,6,6,8,8-H...	20.663	9.1	ng	1675450	5	21.322	3683460	20.0
unknown20.710	20.710	2.2	ng	412535	5	21.322	3683460	20.0
9-Tricosene, (Z)-	21.033	2.1	ng	388487	5	21.322	3683460	20.0