

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
 Data File : BM029522.D
 Acq On : 16 Apr 2021 15:17
 Operator : CG/JU
 Sample : M1947-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 FS-SB9(20-21)

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_M\Methods\8270-BM040121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029522.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.922	3	6	18	rVB	653794	788913	25.50%	3.142%
2	5.269	399	405	415	rBV	1337236	1912800	61.84%	7.617%
3	6.846	666	673	688	rBV	1288723	2056147	66.47%	8.188%
4	7.669	804	813	822	rBV	337220	543225	17.56%	2.163%
5	8.822	1000	1009	1018	rBV	782526	1294865	41.86%	5.157%
6	10.451	1279	1286	1292	rBV	422377	712456	23.03%	2.837%
7	10.504	1292	1295	1300	rVB	47591	69637	2.25%	0.277%
8	12.122	1565	1570	1576	rVB	19414	31783	1.03%	0.127%
9	12.339	1602	1607	1613	rBV2	22900	36217	1.17%	0.144%
10	12.927	1699	1707	1717	rBV	1577762	2342771	75.74%	9.330%
11	13.769	1845	1850	1854	rBV	44425	62103	2.01%	0.247%
12	14.310	1935	1942	1948	rBV2	594404	868657	28.08%	3.459%
13	14.374	1948	1953	1960	rVB	49274	73768	2.38%	0.294%
14	14.710	2006	2010	2019	rBV	31804	52617	1.70%	0.210%
15	14.869	2029	2037	2055	rBV2	62360	280956	9.08%	1.119%
16	15.363	2115	2121	2126	rBV	68829	103198	3.34%	0.411%
17	15.798	2189	2195	2204	rBV	1381927	1967668	63.61%	7.836%
18	16.874	2374	2378	2387	rVB	34920	57703	1.87%	0.230%
19	17.051	2402	2408	2412	rBV	672977	985366	31.86%	3.924%
20	17.092	2412	2415	2422	rVV	454519	644668	20.84%	2.567%
21	17.186	2422	2431	2437	rVV	103292	162556	5.26%	0.647%
22	17.457	2472	2477	2482	rBV	73135	98044	3.17%	0.390%
23	17.927	2553	2557	2559	rBV	46633	62526	2.02%	0.249%
24	17.962	2559	2563	2574	rVB2	443981	648388	20.96%	2.582%
25	18.121	2585	2590	2594	rBV2	71834	132830	4.29%	0.529%
26	18.433	2639	2643	2646	rBV	34909	46073	1.49%	0.183%
27	19.115	2753	2759	2765	rBV	599265	764312	24.71%	3.044%
28	19.174	2765	2769	2773	rVV3	91436	111451	3.60%	0.444%
29	19.245	2777	2781	2788	rVV2	180316	259245	8.38%	1.032%
30	19.445	2811	2815	2816	rBV	63752	74546	2.41%	0.297%
31	19.474	2816	2820	2825	rVB	441907	580111	18.75%	2.310%
32	19.551	2830	2833	2840	rVB7	25534	46964	1.52%	0.187%
33	19.686	2848	2856	2861	rBV	2550744	3093211	100.00%	12.318%
34	19.974	2901	2905	2908	rVB	61536	79159	2.56%	0.315%
35	20.074	2918	2922	2926	rBV	53805	74445	2.41%	0.296%
36	20.956	3068	3072	3078	rBV2	363324	463247	14.98%	1.845%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029522.D
Acq On : 16 Apr 2021 15:17
Operator : CG/JU
Sample : M1947-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB9(20-21)

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_M\Methods\8270-BM040121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.233	3112	3119	3123	rBV2	926210	1465559	47.38%	5.836%
38	21.268	3123	3125	3133	rVB	227894	243517	7.87%	0.970%
39	21.827	3217	3220	3227	rVB4	70161	105828	3.42%	0.421%
40	22.780	3378	3382	3387	rBV	180756	343597	11.11%	1.368%
41	23.339	3473	3477	3484	rVB	165397	307041	9.93%	1.223%
42	23.439	3488	3494	3501	rBV2	590748	1062769	34.36%	4.232%

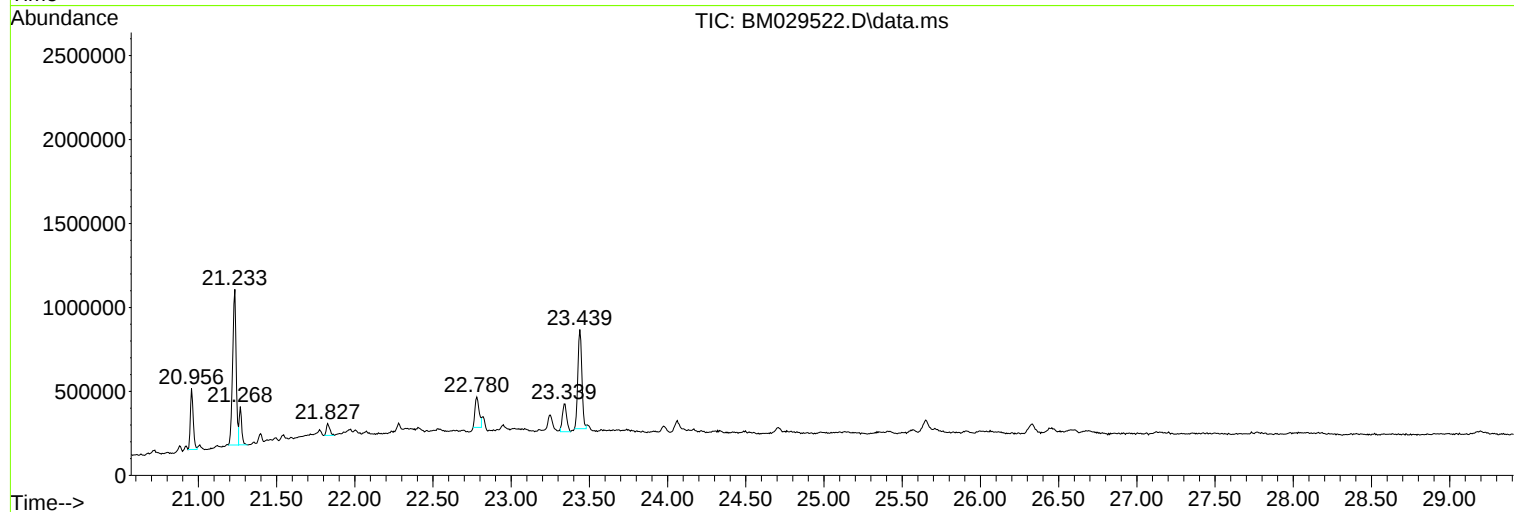
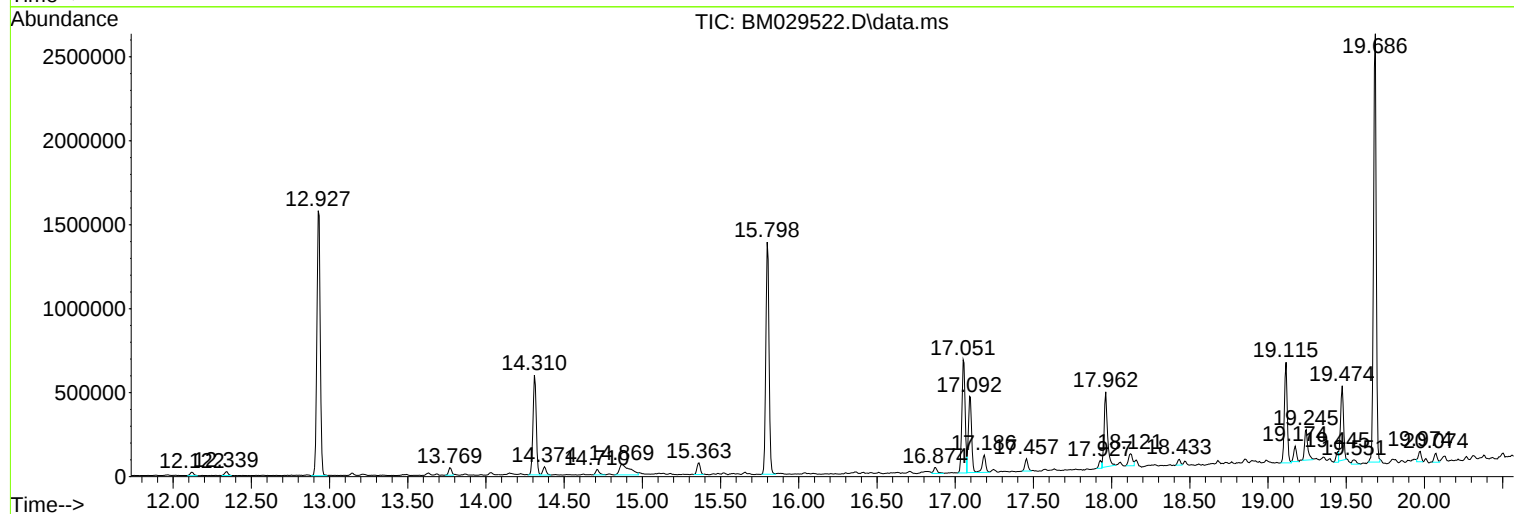
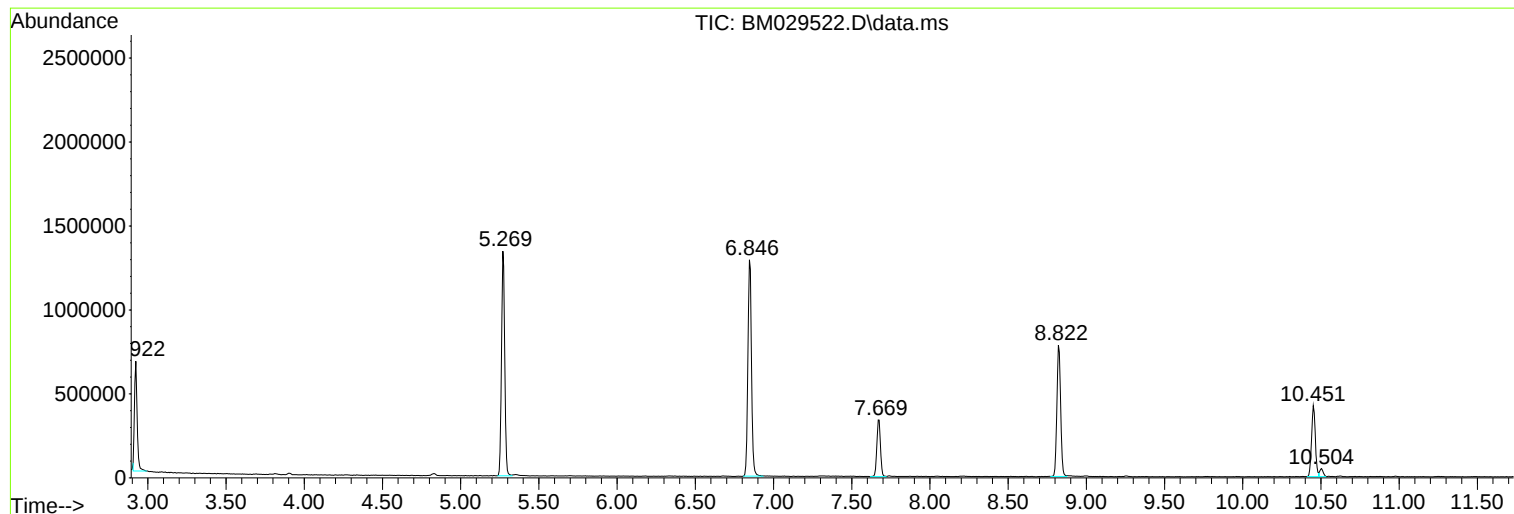
Sum of corrected areas: 25110937

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029522.D
Acq On : 16 Apr 2021 15:17
Operator : CG/JU
Sample : M1947-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB9(20-21)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029522.D
Acq On : 16 Apr 2021 15:17
Operator : CG/JU
Sample : M1947-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB9(20-21)

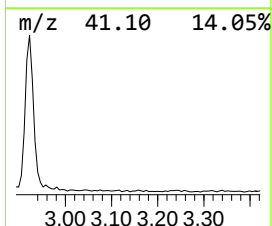
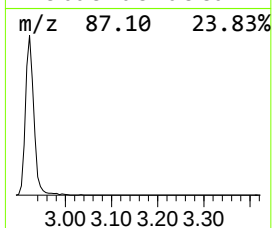
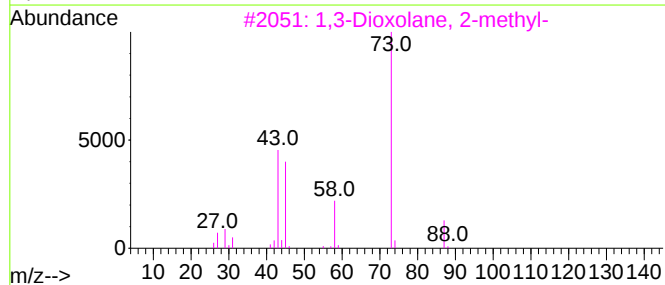
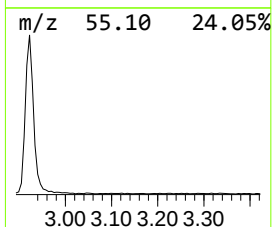
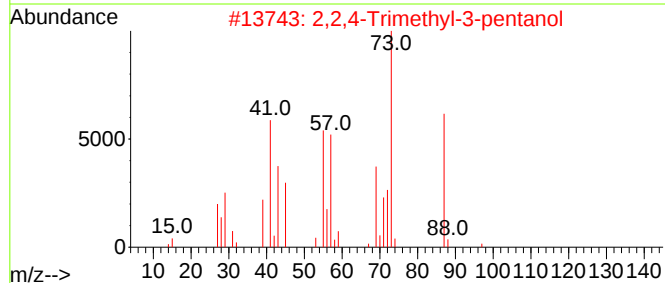
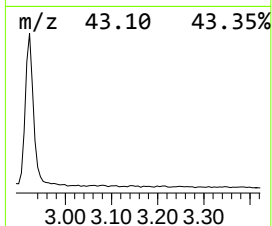
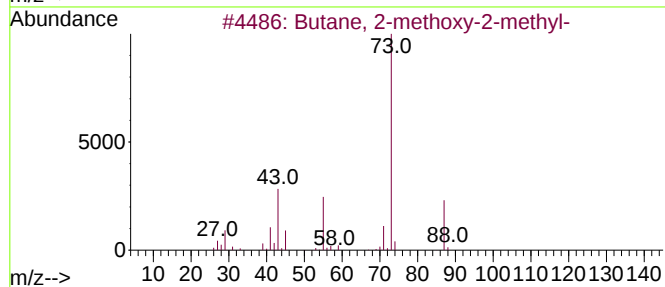
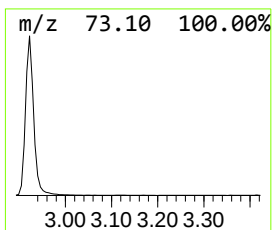
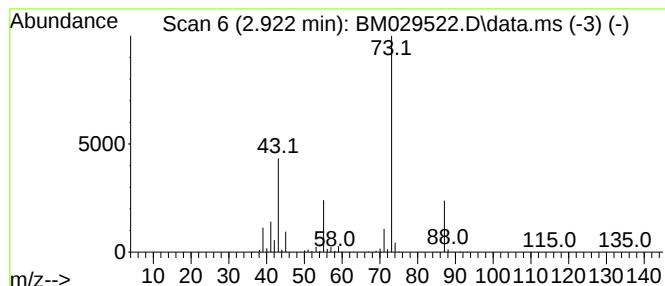
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.922	29.05 ng	788913	1,4-Dichlorobenzene-d4	7.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	50
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029522.D
Acq On : 16 Apr 2021 15:17
Operator : CG/JU
Sample : M1947-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB9(20-21)

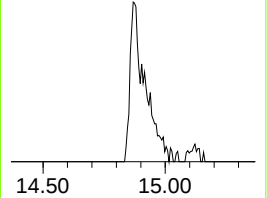
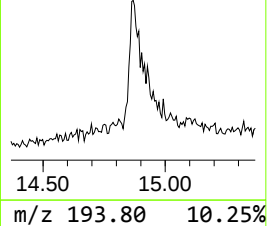
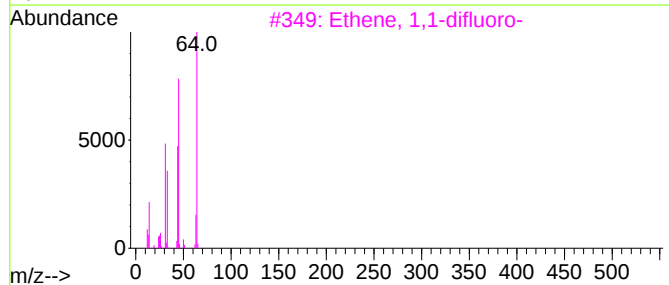
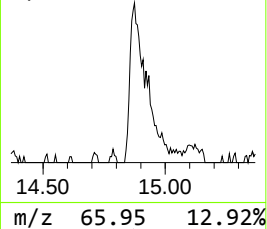
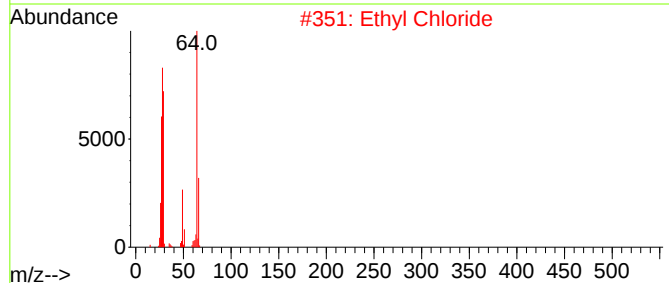
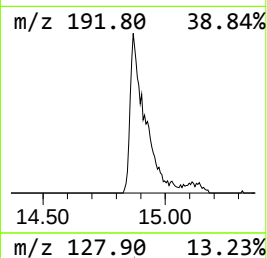
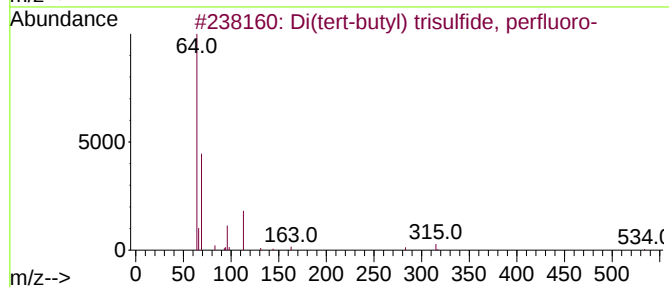
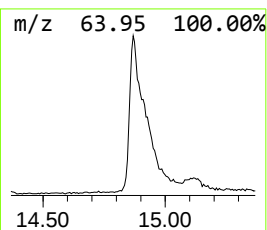
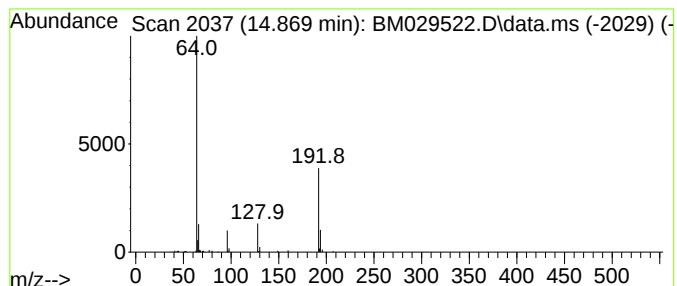
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown14.868 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	6.47 ng	280956	Acenaphthene-d10	14.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	9
2			Ethyl Chloride	64	C2H5Cl	000075-00-3	4
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3
4			Sulfur dioxide	64	O2S	007446-09-5	3
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029522.D
Acq On : 16 Apr 2021 15:17
Operator : CG/JU
Sample : M1947-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB9(20-21)

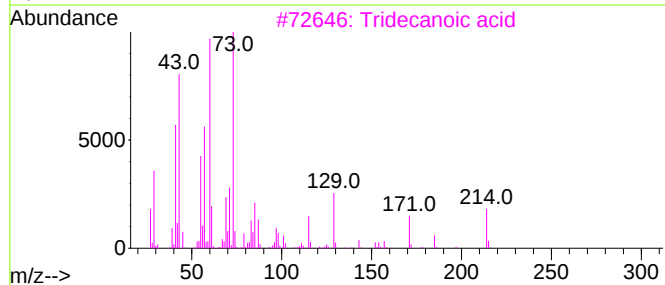
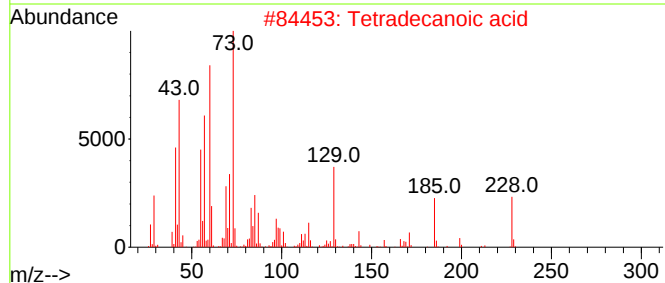
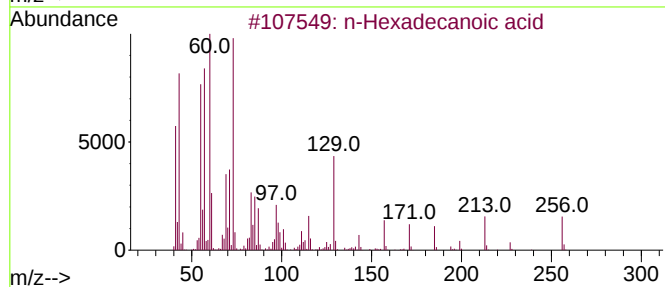
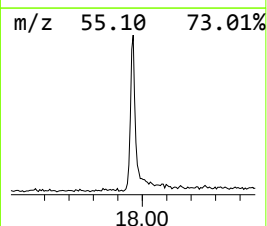
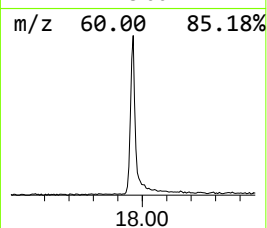
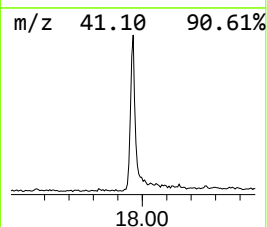
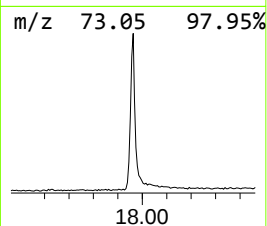
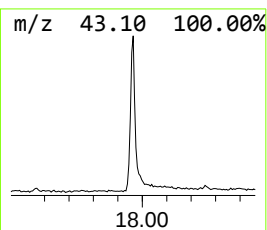
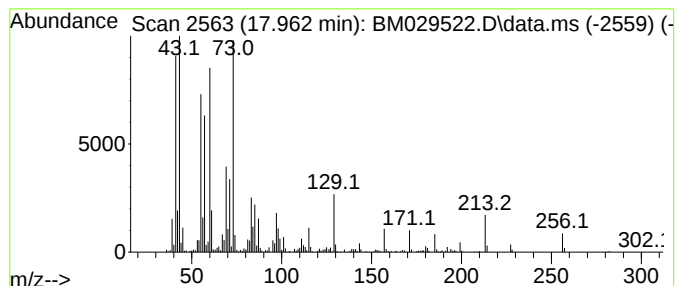
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.962	13.16 ng	648388	Phenanthrene-d10	17.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Dodecanoic acid	200	C12H24O2	000143-07-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029522.D
Acq On : 16 Apr 2021 15:17
Operator : CG/JU
Sample : M1947-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB9(20-21)

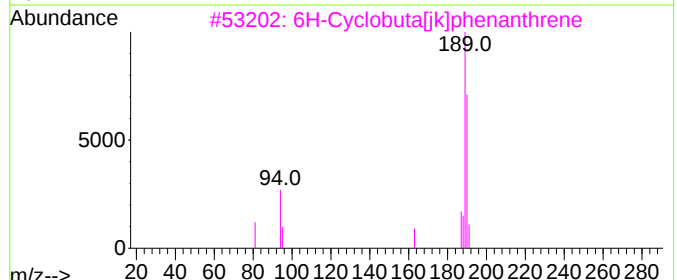
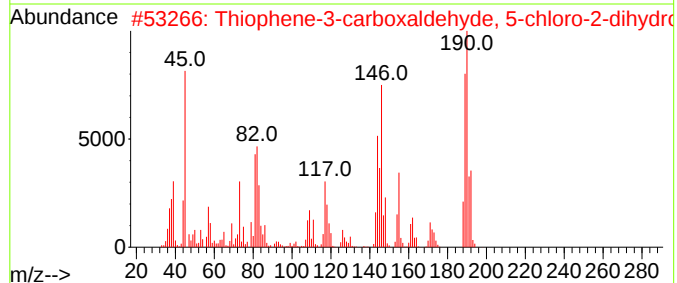
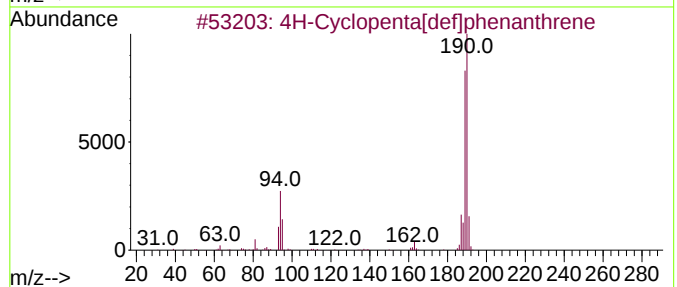
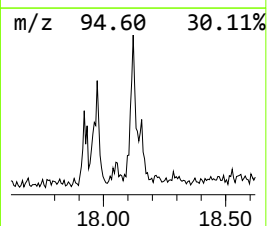
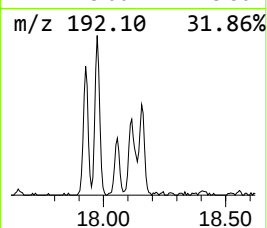
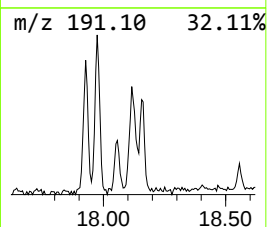
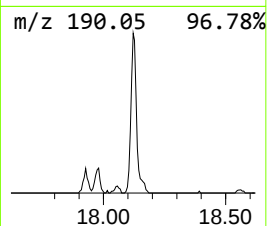
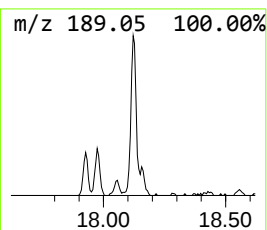
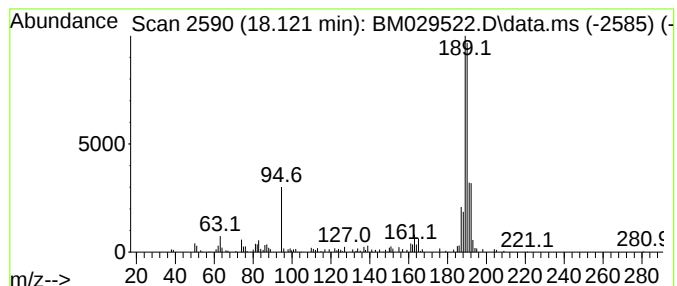
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.121	2.70 ng	132830	Phenanthrene-d10	17.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	80
2			Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	64
3			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	56
4			Methyl diselenide	190	C2H6Se2	007101-31-7	49
5			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029522.D
Acq On : 16 Apr 2021 15:17
Operator : CG/JU
Sample : M1947-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB9(20-21)

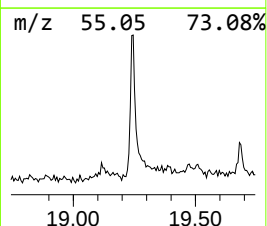
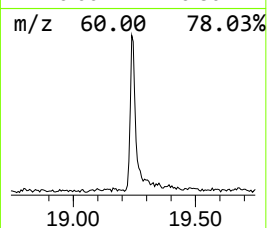
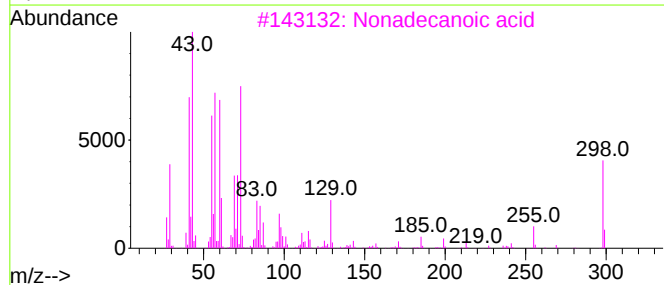
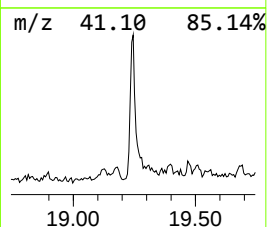
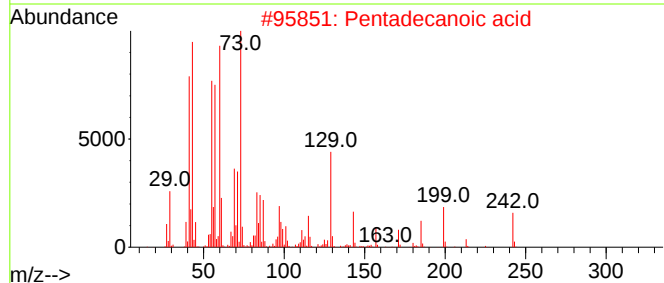
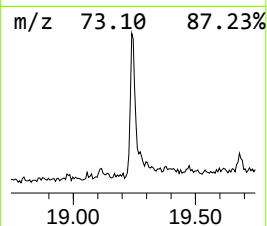
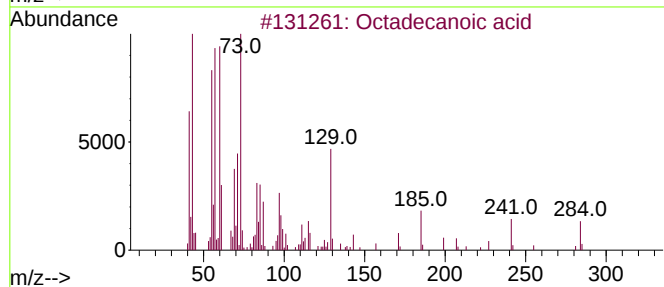
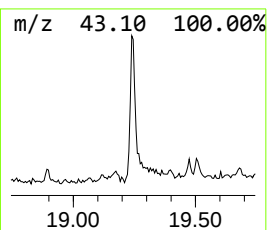
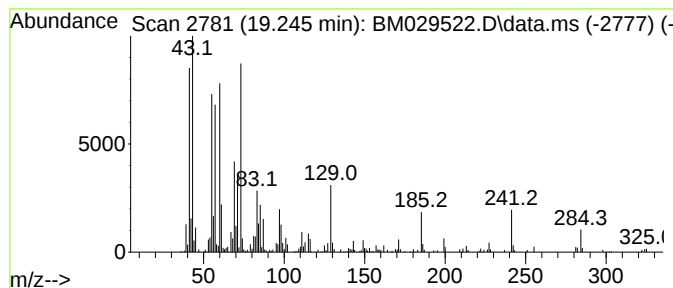
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.245	3.54 ng	259245	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Nonadecanoic acid	298	C19H38O2	000646-30-0	93
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	74
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029522.D
Acq On : 16 Apr 2021 15:17
Operator : CG/JU
Sample : M1947-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB9(20-21)

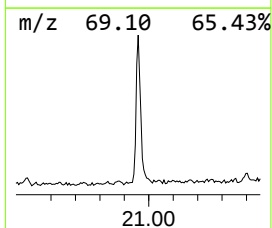
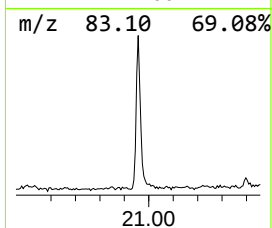
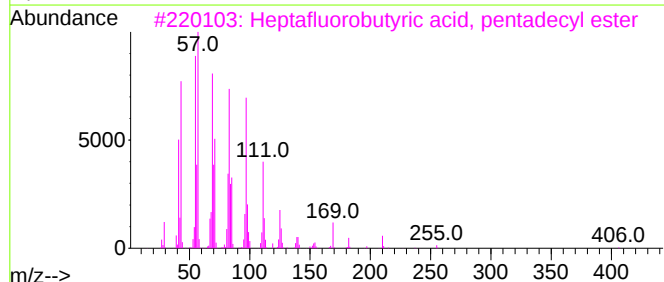
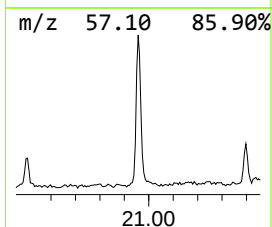
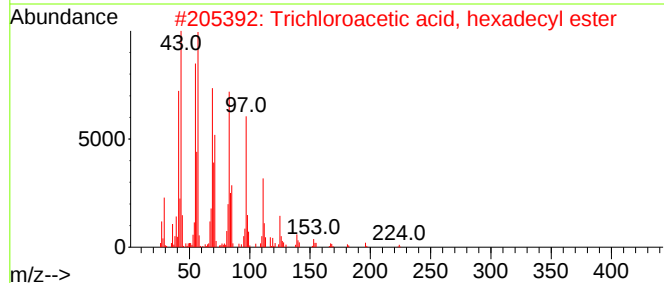
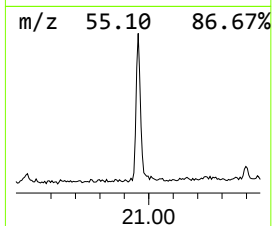
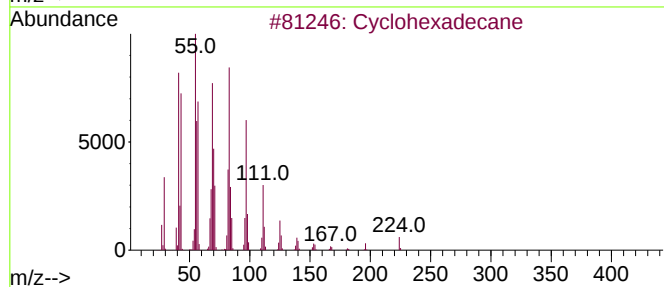
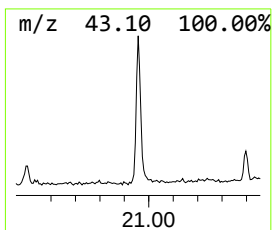
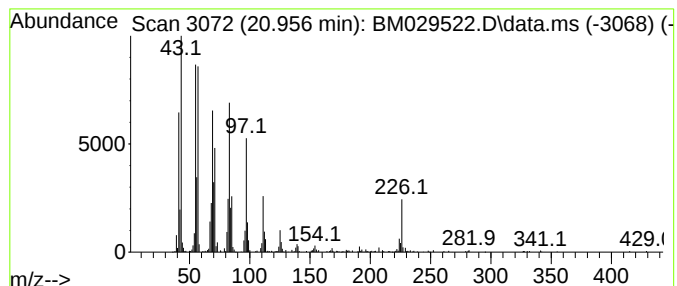
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.956	6.32 ng	463247	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	95
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5			Trichloroacetic acid, 4-hexadecy...	386	C18H33Cl3O2	1000282-92-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029522.D
Acq On : 16 Apr 2021 15:17
Operator : CG/JU
Sample : M1947-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB9(20-21)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.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
Butane, 2-metho...	2.922	29.1	ng	788913	1	7.669	543225	20.0
unknown14.868	14.868	6.5	ng	280956	3	14.310	868657	20.0
n-Hexadecanoic ...	17.962	13.2	ng	648388	4	17.051	985366	20.0
4H-Cyclopenta[d...]	18.121	2.7	ng	132830	4	17.051	985366	20.0
Octadecanoic acid	19.245	3.5	ng	259245	5	21.233	1465560	20.0
Cyclohexadecane	20.956	6.3	ng	463247	5	21.233	1465560	20.0