

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040624\
 Data File : BG060816.D
 Acq On : 6 Apr 2024 18:15
 Operator : MA/JU
 Sample : P1996-07
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP3

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-BG032924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060816.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.106	13	20	27	rBV4	16516	50242	2.31%	0.328%
2	3.188	27	34	48	rVB	225575	516001	23.68%	3.368%
3	3.699	115	121	128	rBV	19257	33866	1.55%	0.221%
4	4.486	250	255	268	rVB	86071	138712	6.37%	0.905%
5	5.080	348	356	362	rBV	23075	36190	1.66%	0.236%
6	5.538	427	434	447	rVB	572396	923558	42.38%	6.027%
7	7.113	694	702	712	rBV	630602	1044556	47.94%	6.817%
8	7.953	838	845	852	rBV	272183	440558	20.22%	2.875%
9	9.104	1032	1041	1052	rBV	389769	679939	31.20%	4.437%
10	10.750	1312	1321	1329	rBV	327997	580633	26.65%	3.789%
11	13.206	1732	1739	1748	rBV	917166	1433788	65.80%	9.357%
12	14.580	1965	1973	1980	rBV	541323	833339	38.24%	5.439%
13	16.067	2219	2226	2238	rBV	776967	1220602	56.02%	7.966%
14	17.324	2434	2440	2445	rBV	663041	1014374	46.55%	6.620%
15	17.365	2445	2447	2453	rVB	56900	71034	3.26%	0.464%
16	17.724	2501	2508	2514	rBV6	13396	25117	1.15%	0.164%
17	18.235	2590	2595	2603	rVB3	116226	173972	7.98%	1.135%
18	18.394	2616	2622	2626	rBV4	18283	33928	1.56%	0.221%
19	19.105	2736	2743	2744	rBV4	15402	25226	1.16%	0.165%
20	19.381	2785	2790	2798	rBV	162172	240393	11.03%	1.569%
21	19.510	2808	2812	2817	rBV3	29718	43963	2.02%	0.287%
22	19.739	2843	2851	2858	rBV	144106	254300	11.67%	1.660%
23	19.951	2879	2887	2894	rBV	1704053	2179010	100.00%	14.221%
24	20.238	2934	2936	2940	rVB3	25972	29830	1.37%	0.195%
25	20.391	2959	2962	2967	rVB3	16825	25034	1.15%	0.163%
26	20.779	3026	3028	3033	rVB2	20708	23816	1.09%	0.155%
27	20.991	3061	3064	3072	rVB3	22895	40536	1.86%	0.265%
28	21.155	3088	3092	3093	rBV3	20692	24736	1.14%	0.161%
29	21.273	3107	3112	3117	rBV6	91739	165897	7.61%	1.083%
30	21.590	3158	3166	3171	rBV2	696658	1287150	59.07%	8.400%
31	22.436	3306	3310	3316	rBV3	50054	78945	3.62%	0.515%
32	23.123	3423	3427	3434	rBV5	46304	104382	4.79%	0.681%
33	23.305	3453	3458	3465	rVB2	124517	238911	10.96%	1.559%
34	23.734	3526	3531	3539	rBV2	48584	144101	6.61%	0.940%
35	23.928	3559	3564	3569	rVB2	48228	101206	4.64%	0.660%
36	24.727	3692	3700	3712	rVB2	401158	1064994	48.88%	6.950%

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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-BG032924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

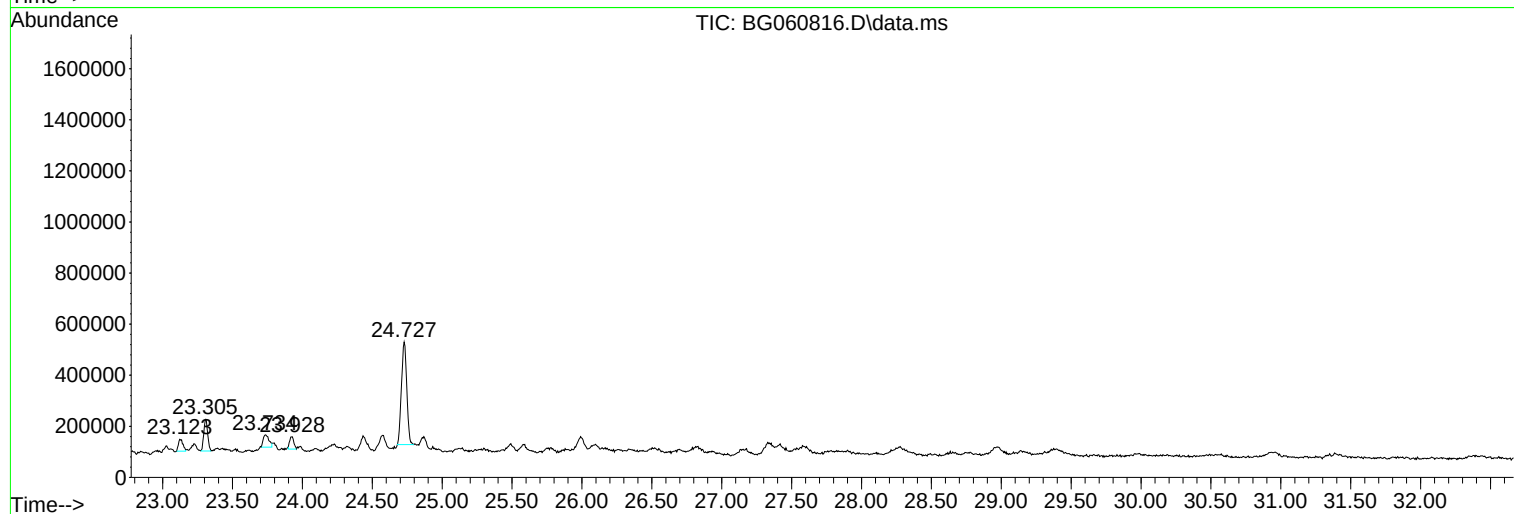
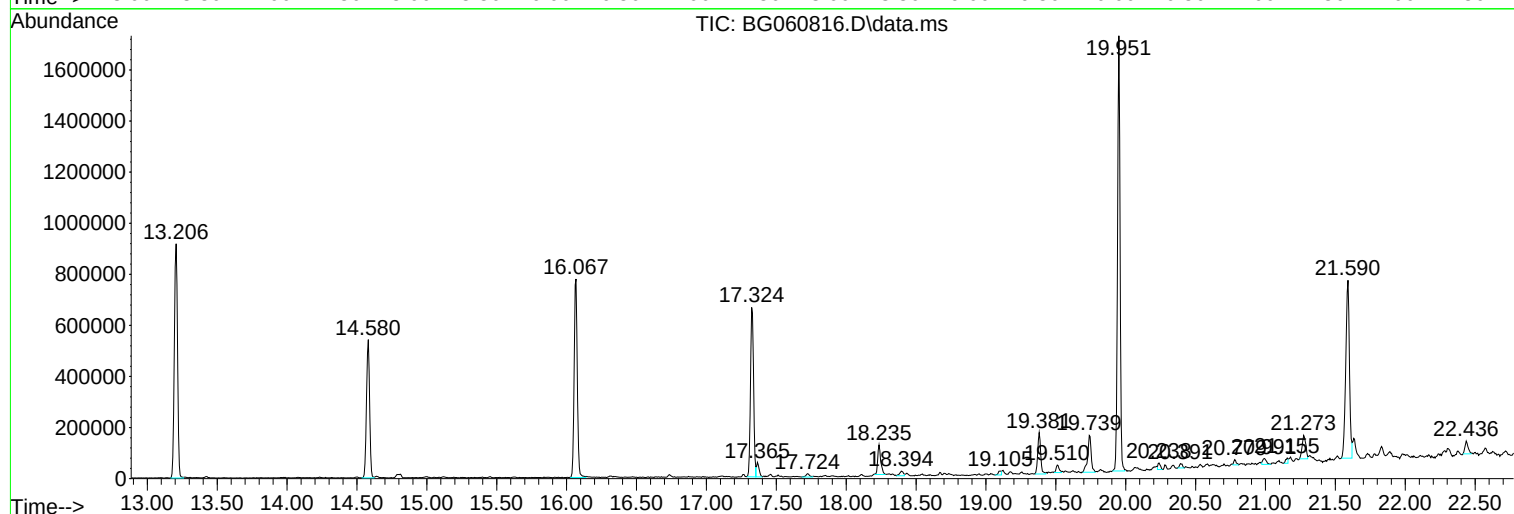
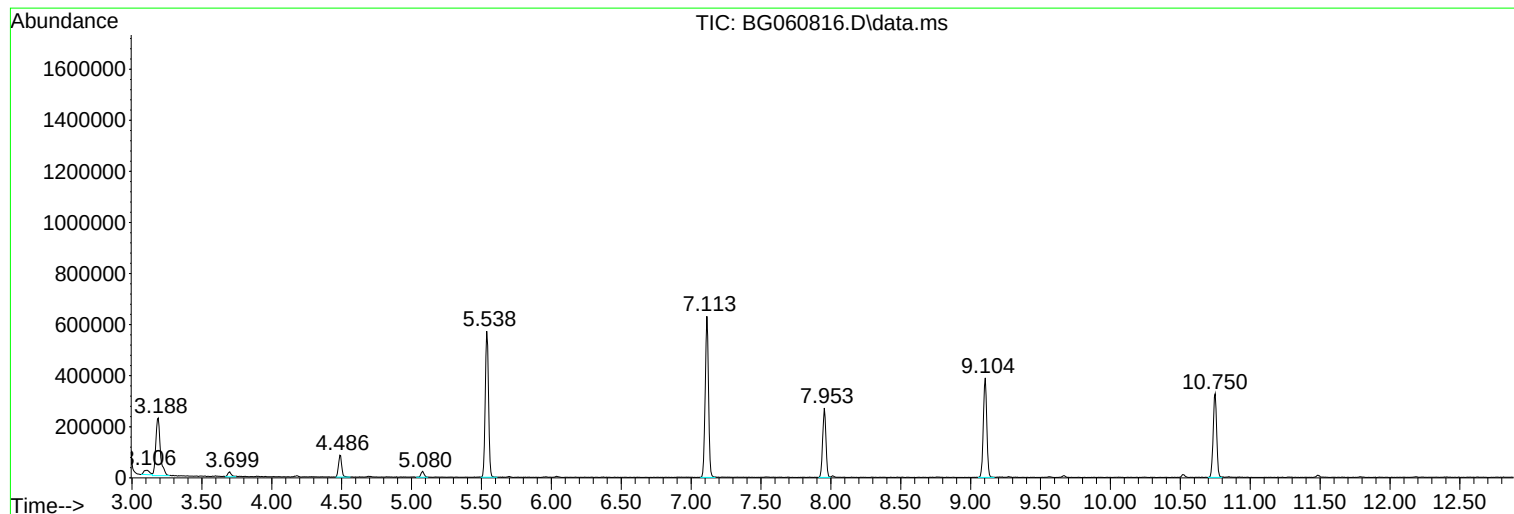
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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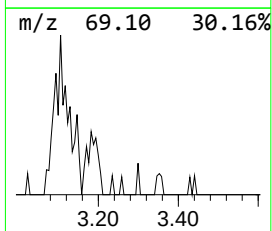
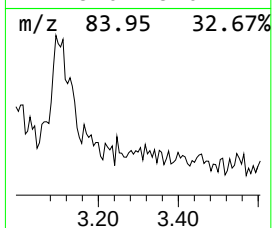
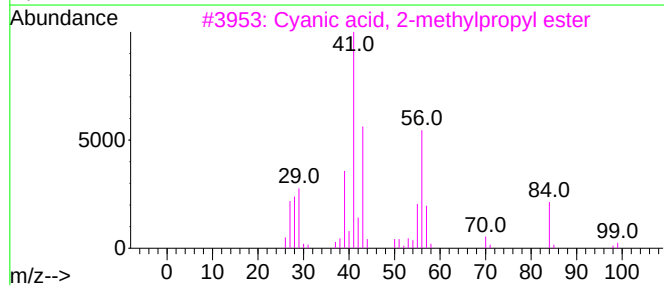
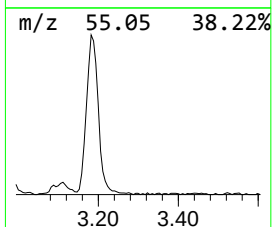
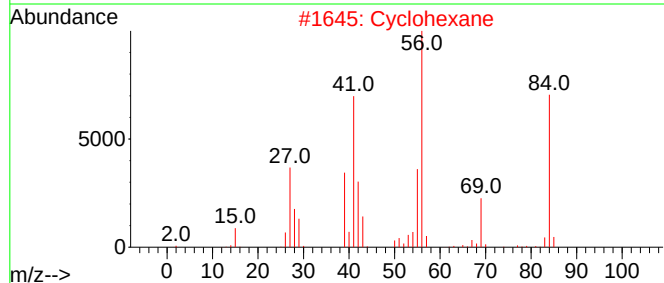
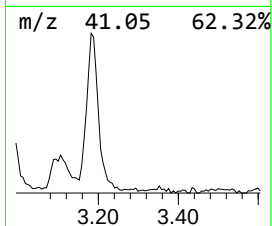
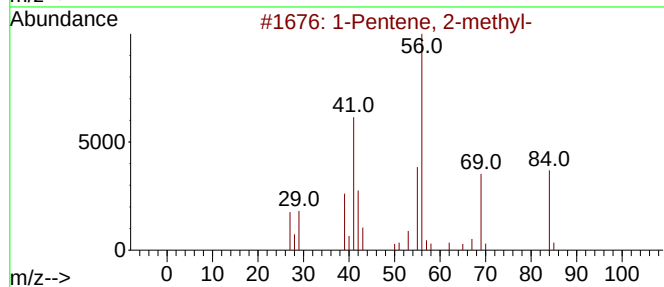
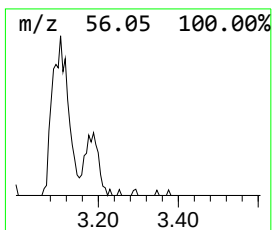
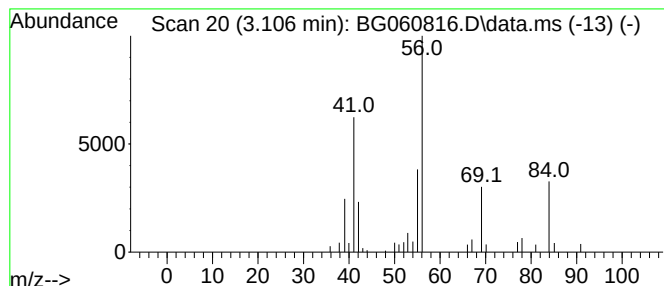
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.106	2.28 ng	50242	1,4-Dichlorobenzene-d4	7.953

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	87
2		Cyclohexane	84	C6H12	000110-82-7	72
3		Cyanic acid, 2-methylpropyl ester	99	C5H9NO	001768-25-8	72
4		Cyclopentane, methyl-	84	C6H12	000096-37-7	64
5		2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	53



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Instrument :
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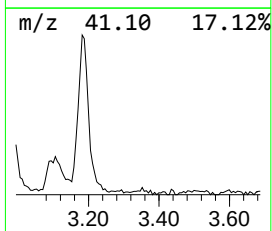
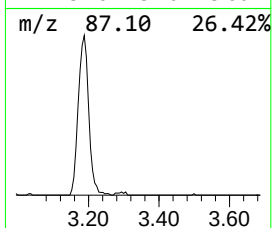
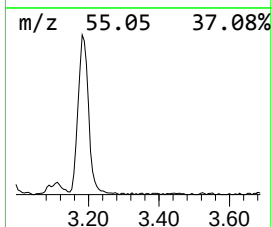
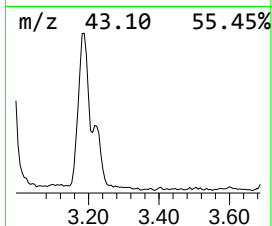
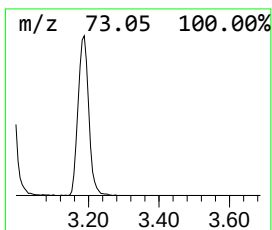
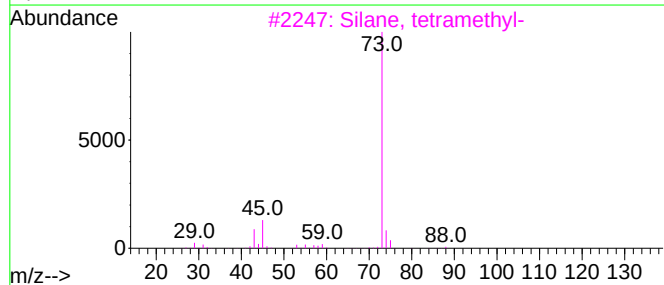
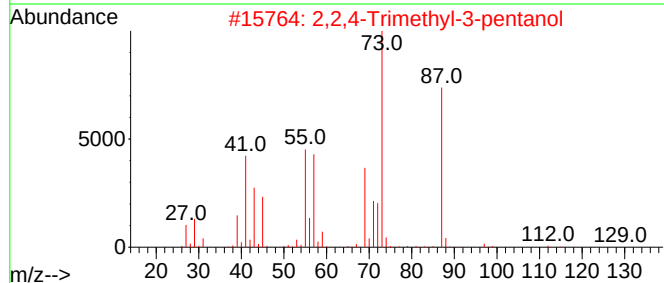
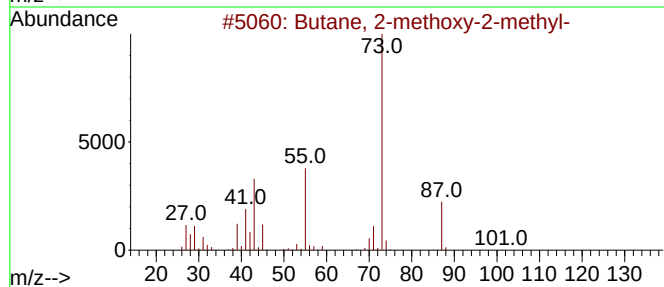
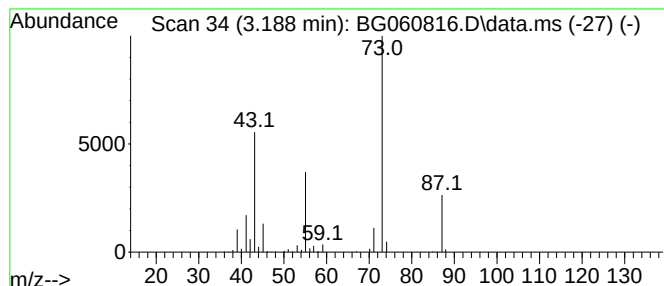
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.188	23.42 ng	516001	1,4-Dichlorobenzene-d4	7.953

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23
5		1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17



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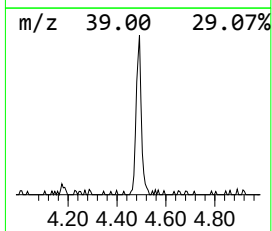
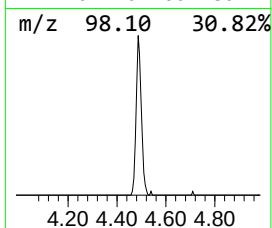
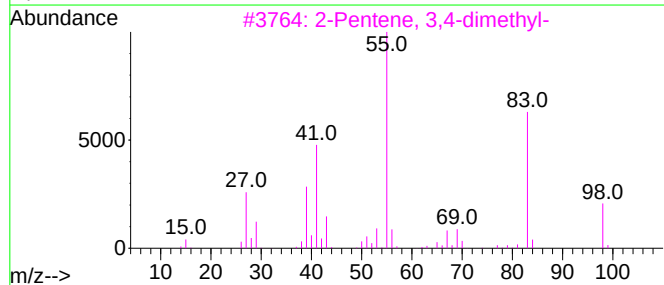
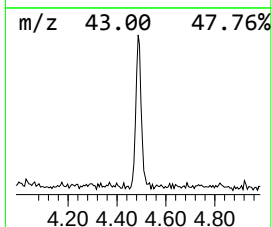
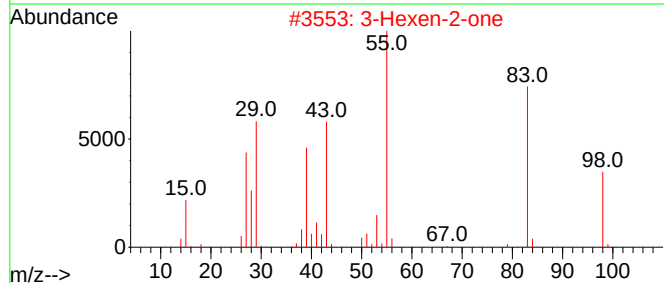
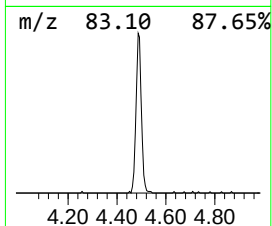
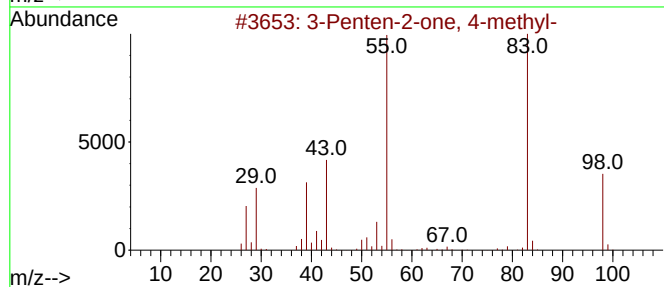
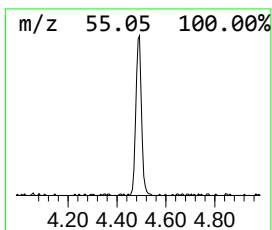
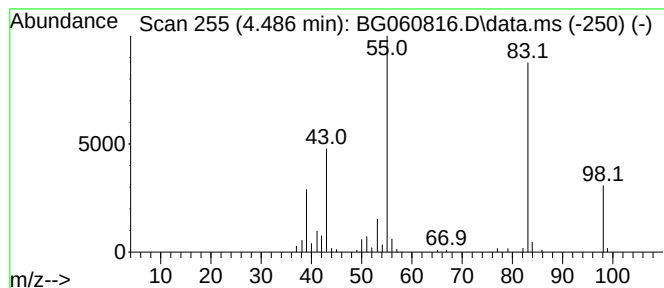
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.486	6.30 ng	138712	1,4-Dichlorobenzene-d4	7.953

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	93
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86
4		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
5		2,4-Azetidinedione, 3,3-diethyl-	141	C7H11N02	042282-85-9	78



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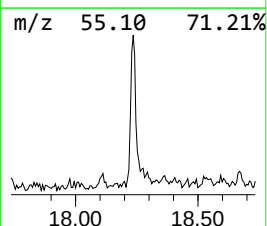
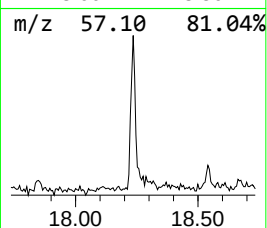
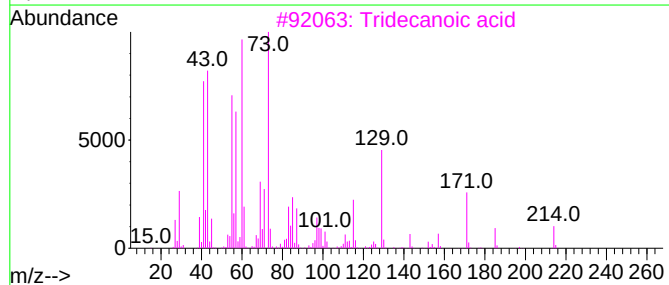
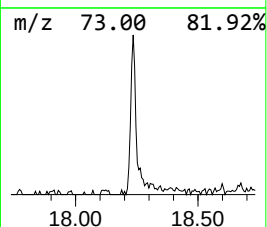
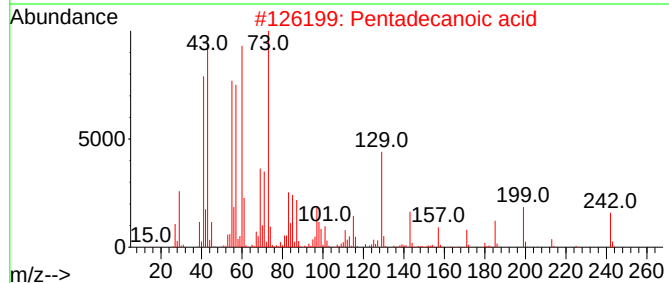
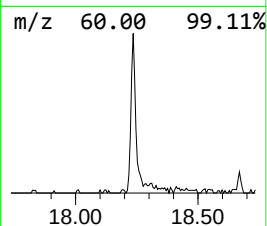
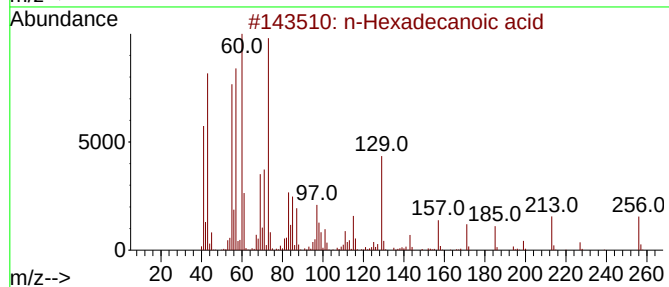
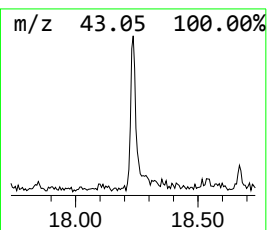
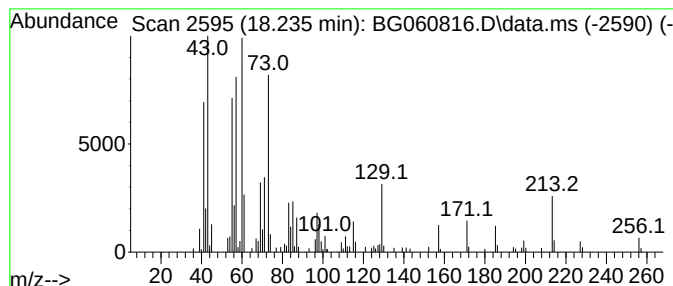
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.235	3.43 ng	173972	Phenanthrene-d10	17.324

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Undecanoic acid	186	C11H22O2	000112-37-8	53
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	53



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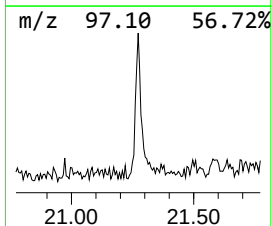
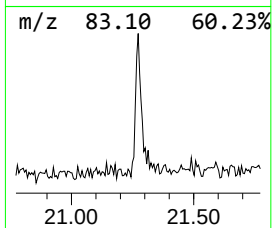
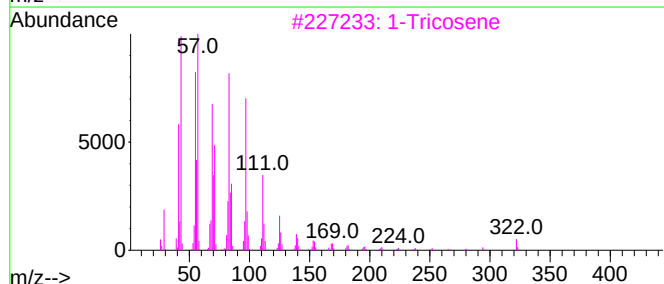
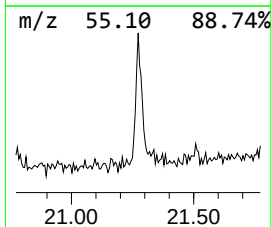
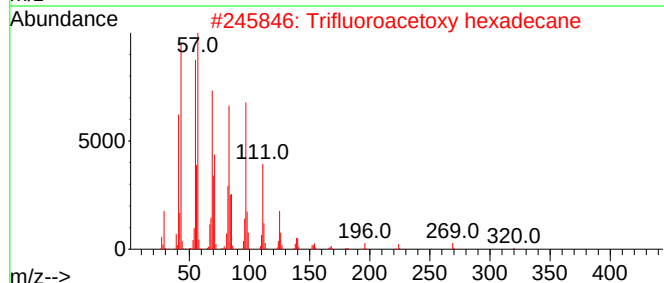
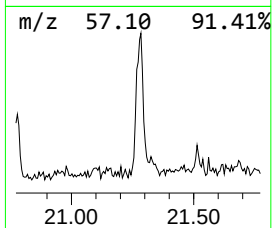
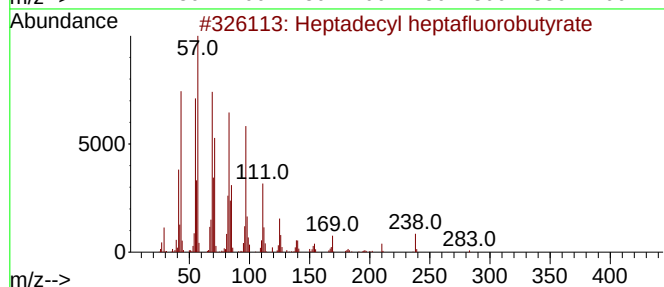
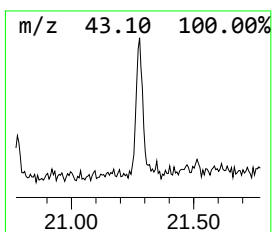
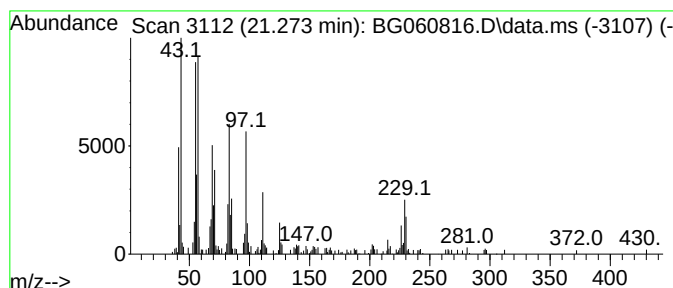
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.273	2.58 ng	165897	Chrysene-d12	21.590

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	89
3			1-Tricosene	322	C23H46	018835-32-0	81
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	81
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040624\
Data File : BG060816.D
Acq On : 6 Apr 2024 18:15
Operator : MA/JU
Sample : P1996-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP3

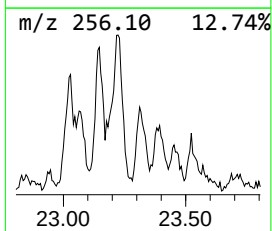
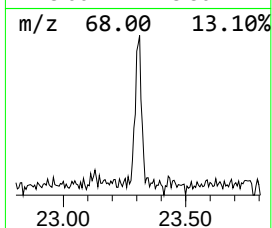
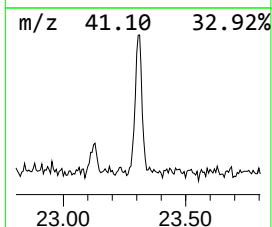
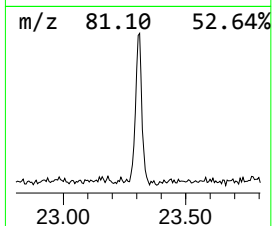
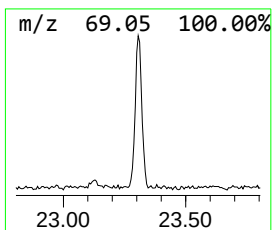
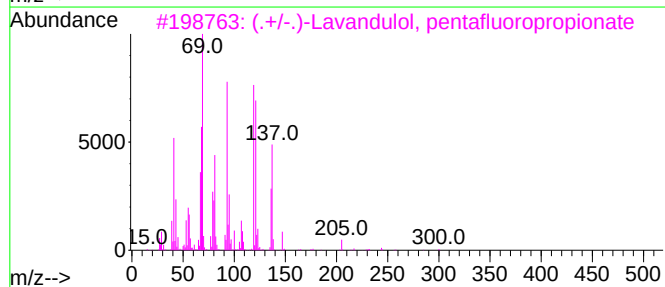
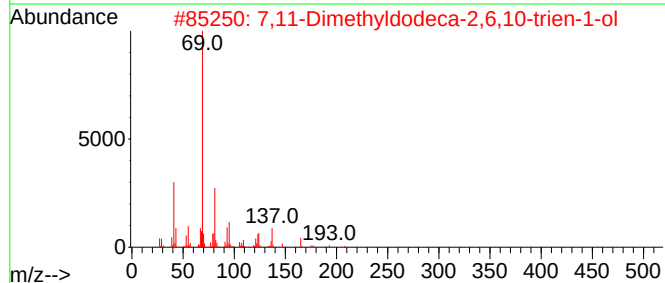
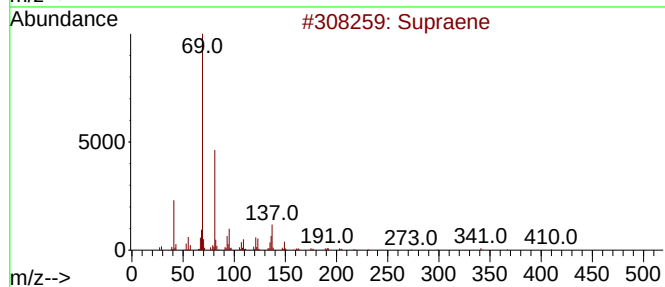
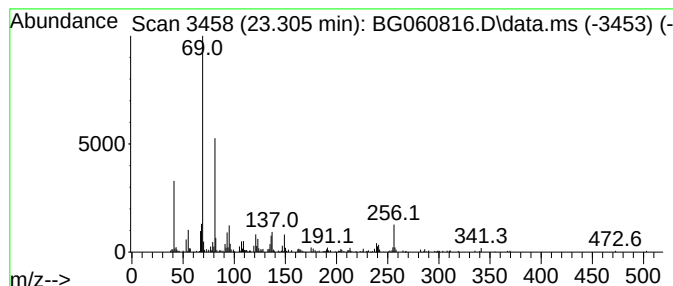
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.305	4.49 ng	238911	Perylene-d12	24.727

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	74
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
3			(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	64
4			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59
5			6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040624\
Data File : BG060816.D
Acq On : 6 Apr 2024 18:15
Operator : MA/JU
Sample : P1996-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Pentene, 2-me...	3.106	2.3	ng	50242	1	7.953	440558	20.0
Butane, 2-metho...	3.188	23.4	ng	516001	1	7.953	440558	20.0
3-Penten-2-one,...	4.486	6.3	ng	138712	1	7.953	440558	20.0
n-Hexadecanoic ...	18.235	3.4	ng	173972	4	17.324	1014370	20.0
Heptadecyl hept...	21.273	2.6	ng	165897	5	21.590	1287150	20.0
Supraene	23.305	4.5	ng	238911	6	24.727	1064990	20.0