

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040224\
 Data File : BG060752.D
 Acq On : 3 Apr 2024 00:50
 Operator : MA/JU
 Sample : P1879-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EB-01(0-2)

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: BG060752.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.094	13	18	27	rBV5	27041	73870	2.15%	0.302%
2	3.176	27	32	47	rVB	302994	553444	16.10%	2.260%
3	3.687	114	119	132	rVB	53769	90130	2.62%	0.368%
4	5.538	427	434	445	rVB	881384	1410489	41.04%	5.760%
5	7.113	693	702	711	rBV	921853	1546495	44.99%	6.315%
6	7.953	836	845	852	rBV	285146	484904	14.11%	1.980%
7	9.104	1032	1041	1049	rBV	531942	922596	26.84%	3.767%
8	9.668	1128	1137	1143	rBV2	30249	53480	1.56%	0.218%
9	10.749	1314	1321	1328	rBV	379853	660559	19.22%	2.697%
10	11.484	1440	1446	1454	rBV3	20948	38162	1.11%	0.156%
11	13.205	1732	1739	1748	rBV	1341737	2103159	61.19%	8.588%
12	14.580	1966	1973	1981	rBV	632486	1008546	29.34%	4.118%
13	14.792	2004	2009	2011	rBV3	24447	35050	1.02%	0.143%
14	15.479	2119	2126	2131	rBV7	19432	34696	1.01%	0.142%
15	16.067	2219	2226	2236	rBV	1185833	1783872	51.90%	7.284%
16	17.330	2434	2441	2445	rBV	779952	1163598	33.85%	4.751%
17	17.371	2445	2448	2456	rVV	147083	220340	6.41%	0.900%
18	17.453	2457	2462	2468	rVB3	23105	52065	1.51%	0.213%
19	18.205	2587	2590	2592	rBV	40312	48853	1.42%	0.199%
20	18.241	2592	2596	2607	rVB3	464341	698494	20.32%	2.852%
21	18.399	2618	2623	2627	rBV3	53749	96643	2.81%	0.395%
22	18.435	2627	2629	2634	rVB2	36733	45315	1.32%	0.185%
23	18.711	2672	2676	2678	rBV	24426	36872	1.07%	0.151%
24	19.116	2739	2745	2750	rBV4	47573	113954	3.32%	0.465%
25	19.181	2753	2756	2759	rVV4	31569	45445	1.32%	0.186%
26	19.216	2759	2762	2765	rVV4	32610	38175	1.11%	0.156%
27	19.263	2766	2770	2774	rVB5	48911	76331	2.22%	0.312%
28	19.381	2785	2790	2800	rBV	288972	536513	15.61%	2.191%
29	19.516	2809	2813	2821	rBV3	162197	247710	7.21%	1.012%
30	19.745	2847	2852	2857	rVB	281467	397907	11.58%	1.625%
31	19.956	2882	2888	2897	rVB	2732054	3437053	100.00%	14.035%
32	20.238	2934	2936	2942	rVB4	69034	91429	2.66%	0.373%
33	20.397	2961	2963	2967	rVB	57427	59181	1.72%	0.242%
34	20.538	2984	2987	2990	rVB2	46231	52282	1.52%	0.213%
35	20.656	3003	3007	3012	rVB	385057	444677	12.94%	1.816%
36	21.278	3109	3113	3125	rVB5	266903	521783	15.18%	2.131%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040224\
Data File : BG060752.D
Acq On : 3 Apr 2024 00:50
Operator : MA/JU
Sample : P1879-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB-01(0-2)

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

37	21.525	3150	3155	3159	rBV	625981	831948	24.21%	3.397%
38	21.590	3159	3166	3171	rVV3	818919	1571737	45.73%	6.418%
39	21.637	3172	3174	3181	rVB	185136	256996	7.48%	1.049%
40	22.453	3308	3313	3320	rBV2	200677	356823	10.38%	1.457%
41	23.946	3560	3567	3572	rBV	435504	992094	28.86%	4.051%
42	24.733	3693	3701	3710	rVB	467354	1255574	36.53%	5.127%

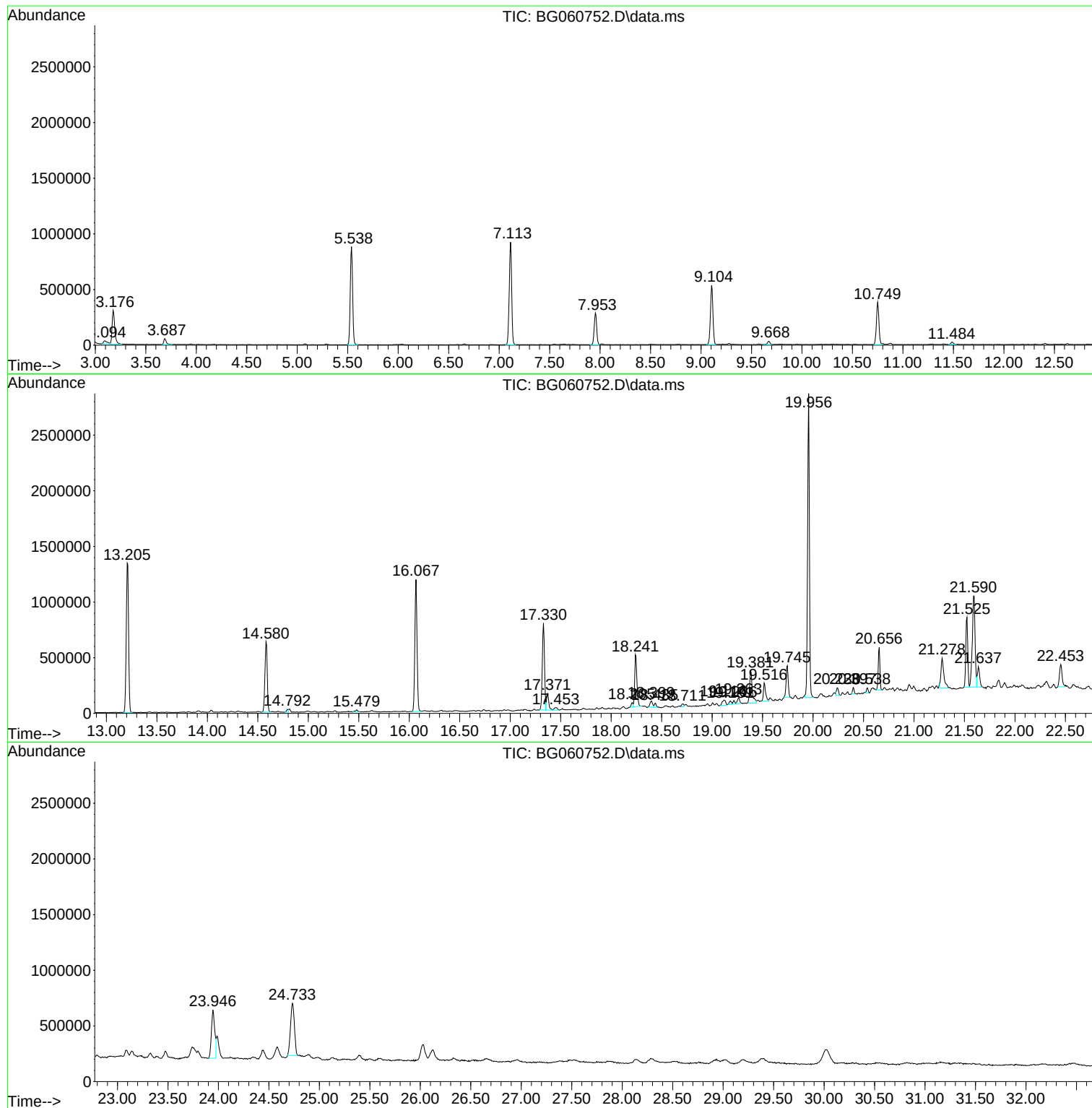
Sum of corrected areas: 24489244

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040224\
Data File : BG060752.D
Acq On : 3 Apr 2024 00:50
Operator : MA/JU
Sample : P1879-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB-01(0-2)

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040224\
Data File : BG060752.D
Acq On : 3 Apr 2024 00:50
Operator : MA/JU
Sample : P1879-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB-01(0-2)

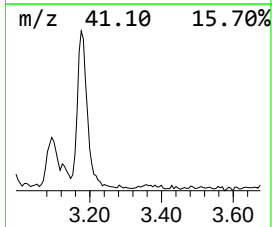
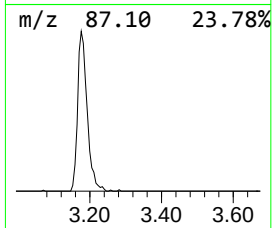
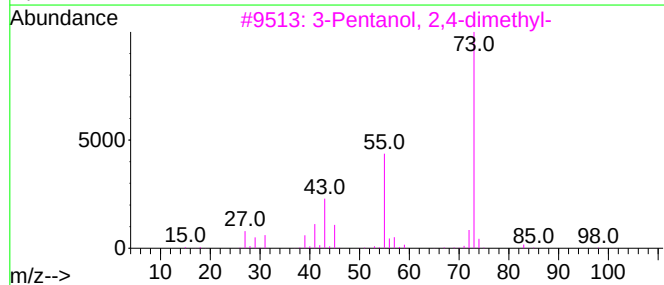
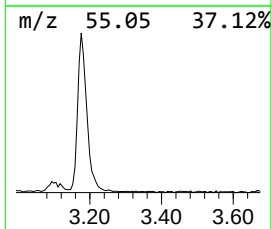
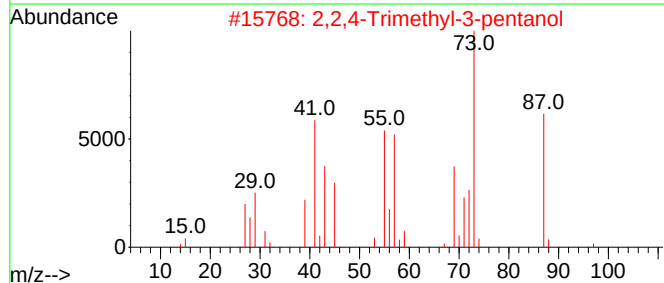
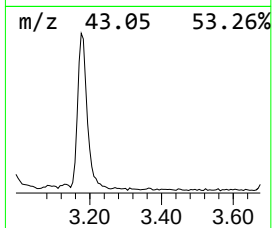
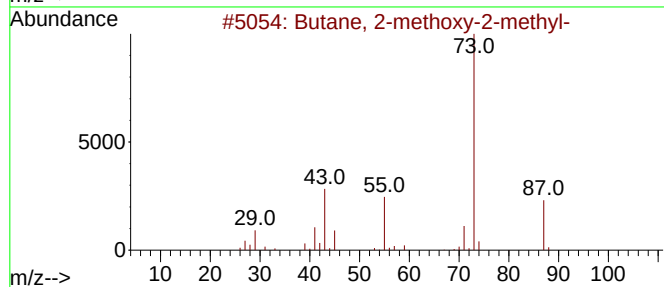
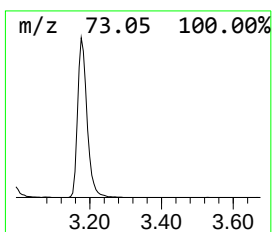
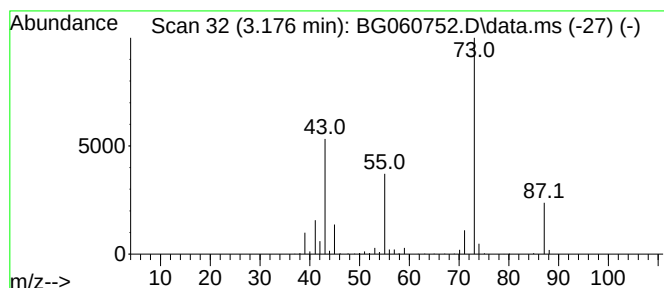
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.176	22.83 ng	553444	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	43
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040224\
Data File : BG060752.D
Acq On : 3 Apr 2024 00:50
Operator : MA/JU
Sample : P1879-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB-01(0-2)

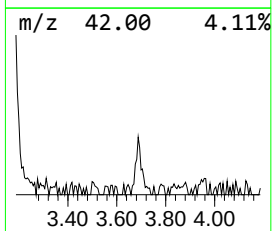
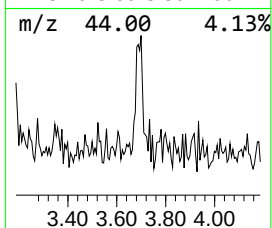
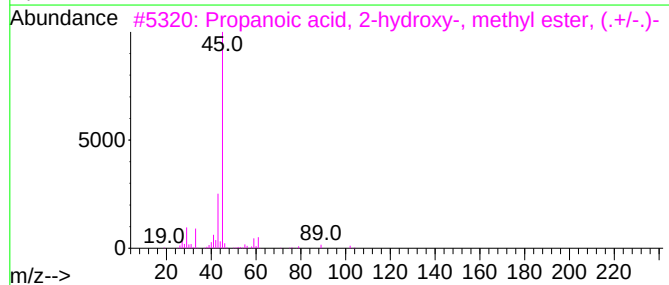
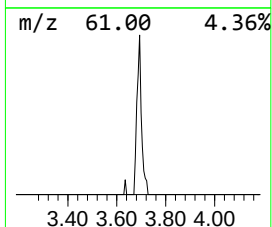
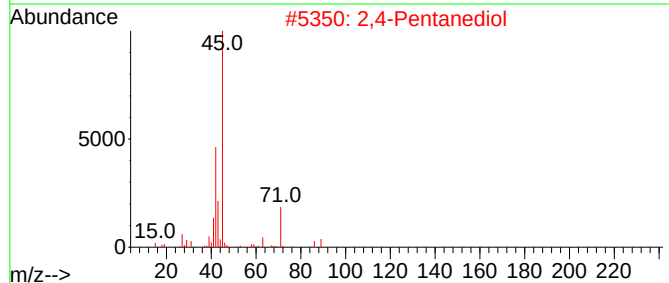
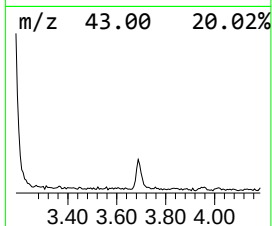
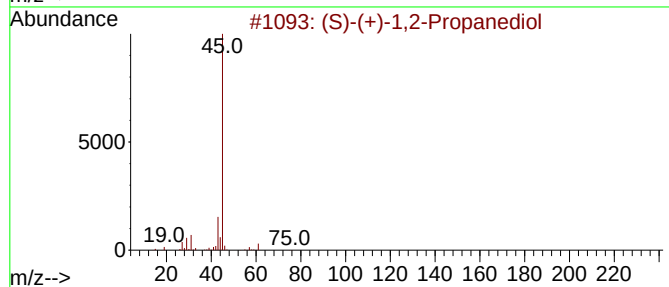
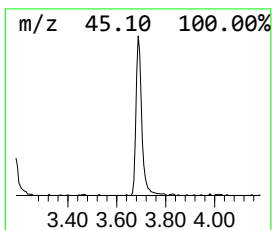
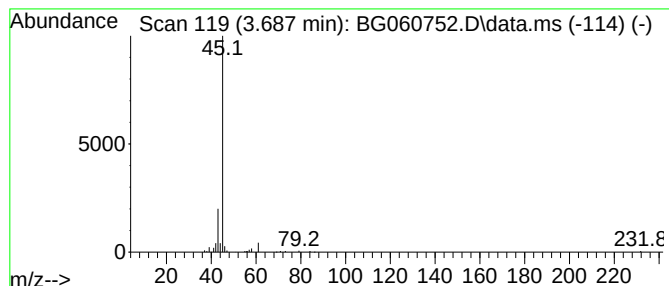
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown3.687 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.687	3.72 ng	90130	1,4-Dichlorobenzene-d4	7.953

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	9
2	2,4-Pentanediol			104	C5H12O2	000625-69-4	9
3	Propanoic acid, 2-hydroxy-, meth...			104	C4H8O3	000547-64-8	9
4	(2R,4R)-(-)-Pentanediol			104	C5H12O2	042075-32-1	9
5	Propylene Glycol			76	C3H8O2	000057-55-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040224\
Data File : BG060752.D
Acq On : 3 Apr 2024 00:50
Operator : MA/JU
Sample : P1879-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB-01(0-2)

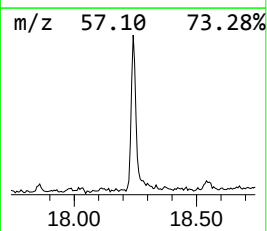
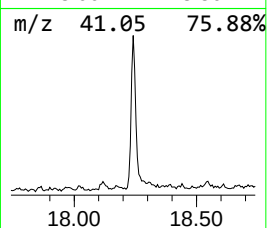
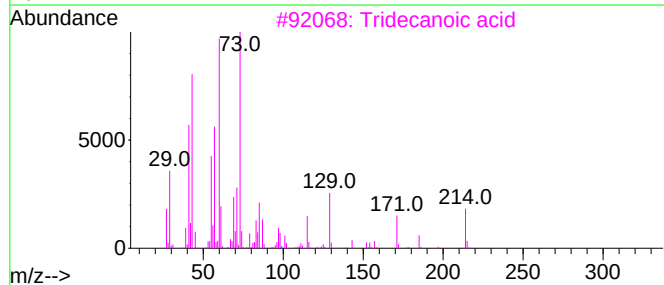
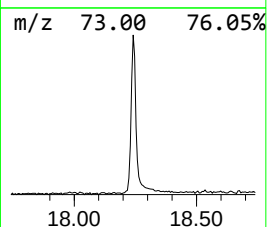
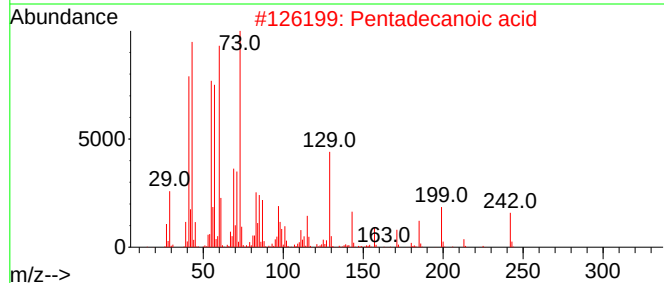
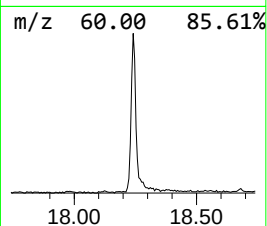
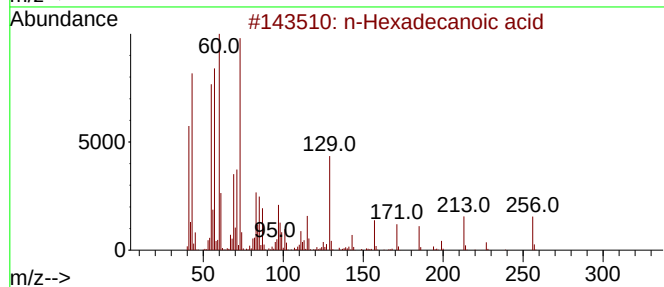
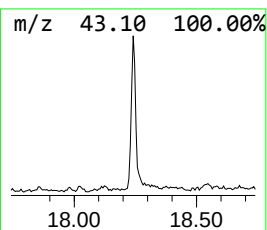
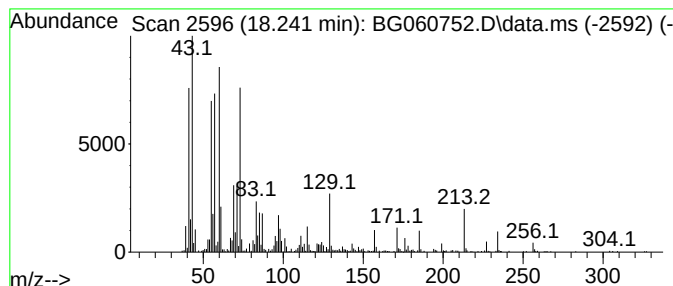
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.241	12.01 ng	698494	Phenanthrene-d10	17.330

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3			Tridecanoic acid	214	C13H26O2	000638-53-9	68
4			Nonanoic acid	158	C9H18O2	000112-05-0	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040224\
Data File : BG060752.D
Acq On : 3 Apr 2024 00:50
Operator : MA/JU
Sample : P1879-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB-01(0-2)

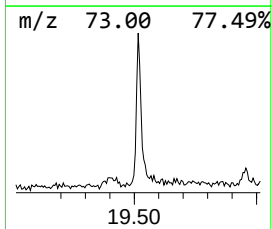
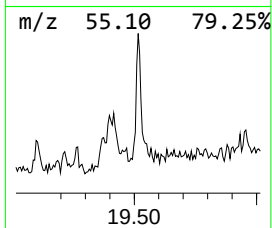
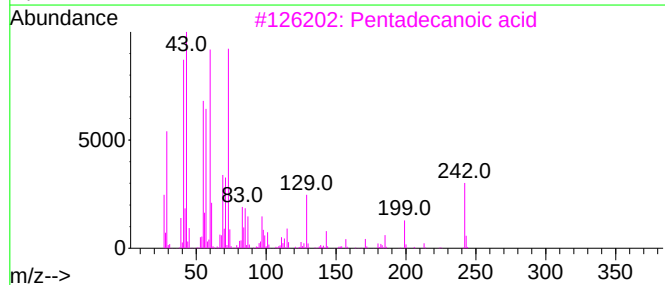
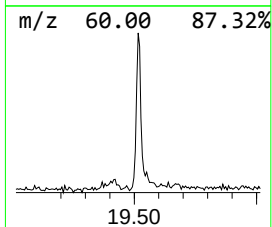
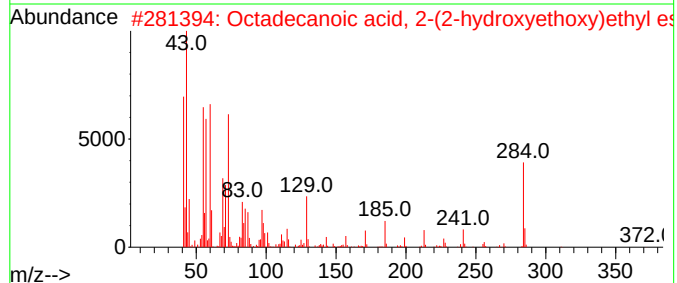
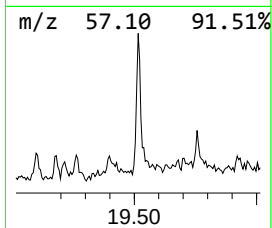
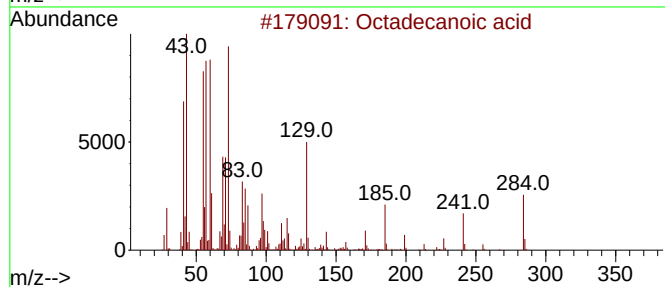
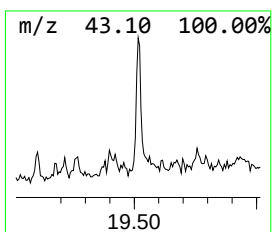
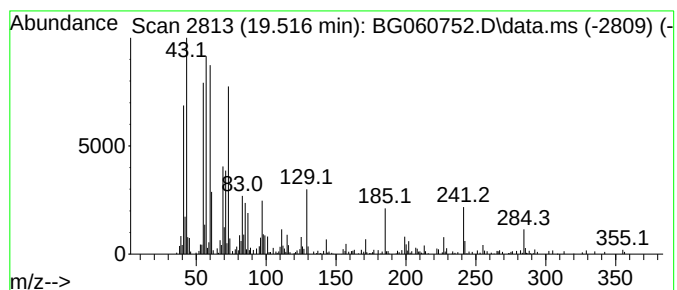
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.516	3.15 ng	247710	Chrysene-d12	21.596

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040224\
Data File : BG060752.D
Acq On : 3 Apr 2024 00:50
Operator : MA/JU
Sample : P1879-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB-01(0-2)

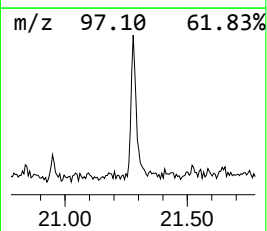
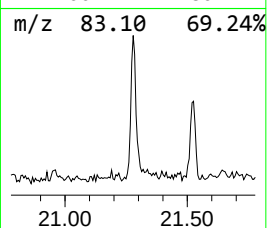
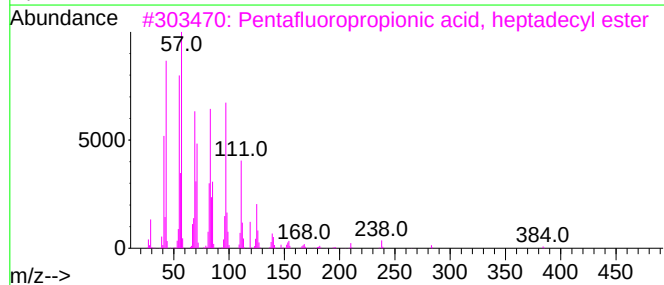
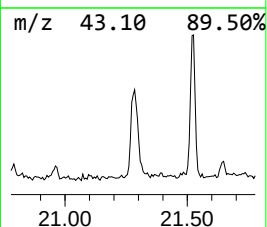
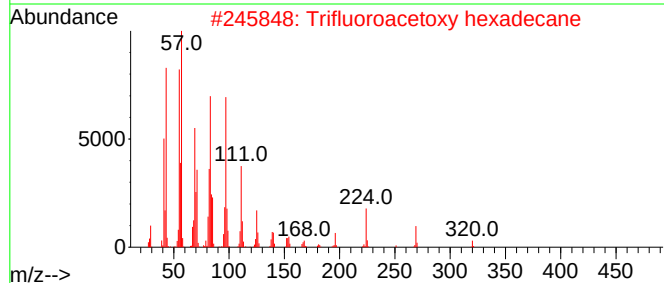
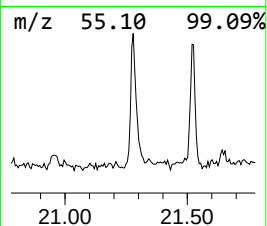
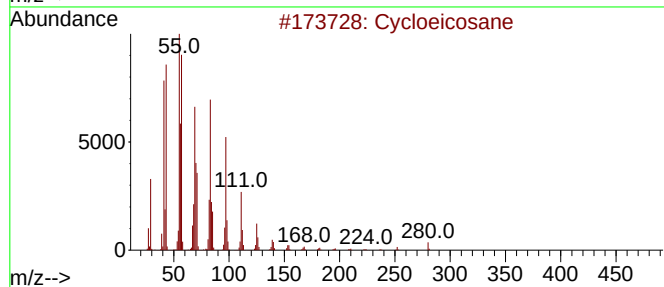
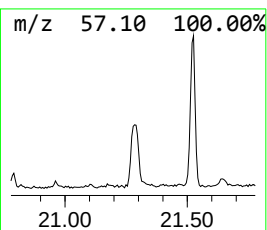
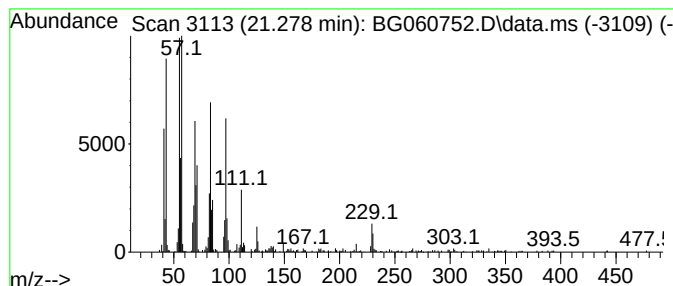
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cycloeicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.278	6.64 ng	521783	Chrysene-d12	21.596

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	91
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
4			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90
5			1-Docosene	308	C22H44	001599-67-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040224\
Data File : BG060752.D
Acq On : 3 Apr 2024 00:50
Operator : MA/JU
Sample : P1879-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB-01(0-2)

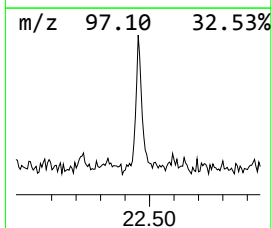
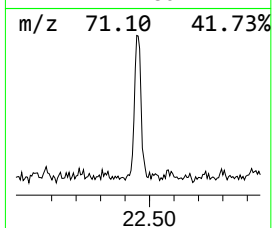
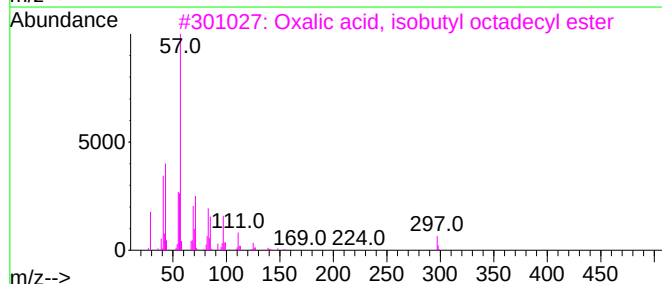
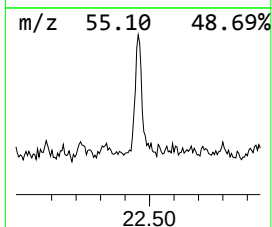
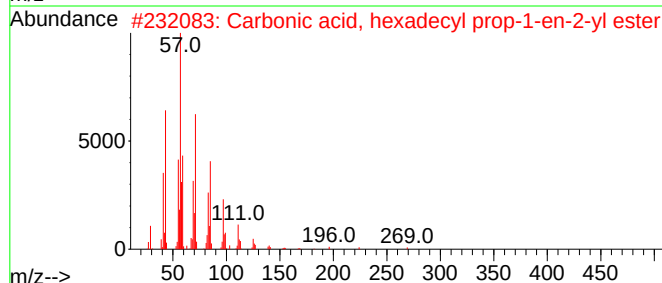
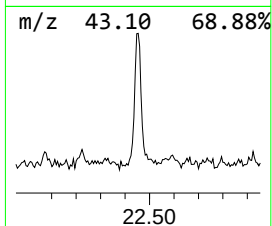
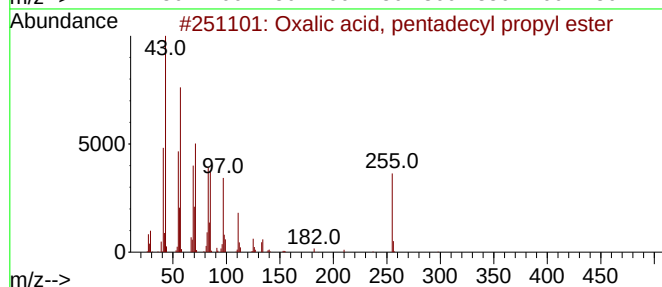
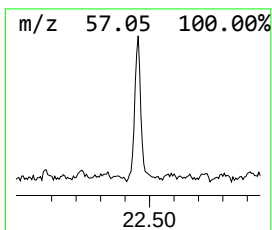
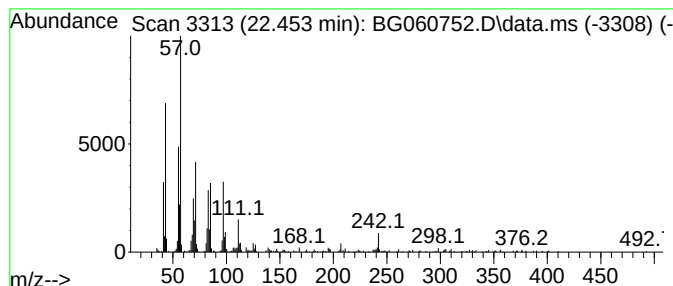
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxalic acid, pentadecyl pro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.453	4.54 ng	356823	Chrysene-d12	21.596

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	80
2			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	72
3			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	68
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	68
5			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040224\
Data File : BG060752.D
Acq On : 3 Apr 2024 00:50
Operator : MA/JU
Sample : P1879-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB-01(0-2)

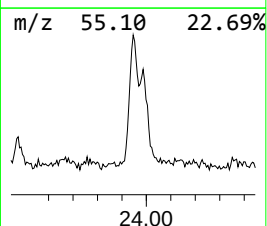
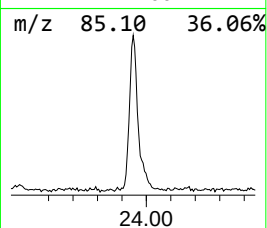
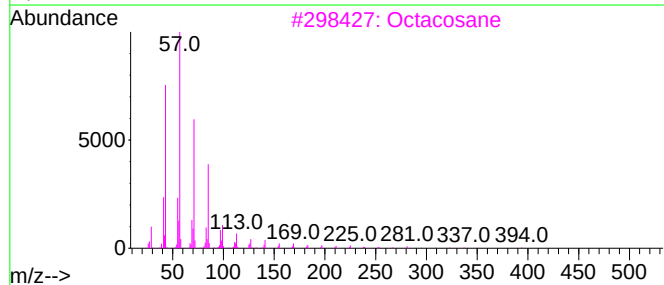
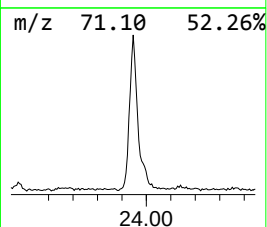
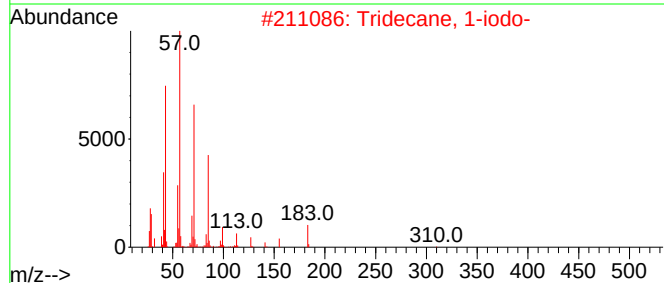
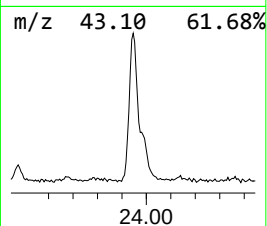
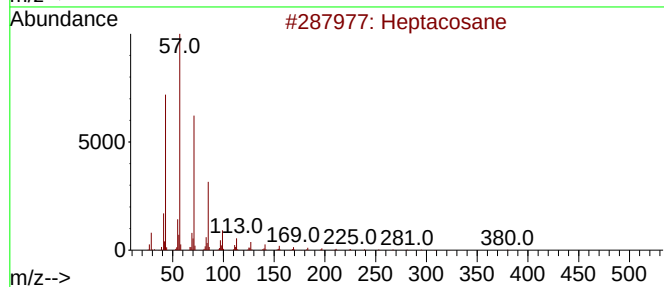
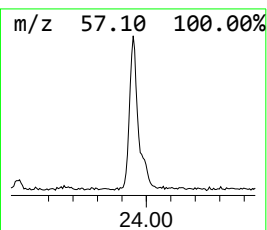
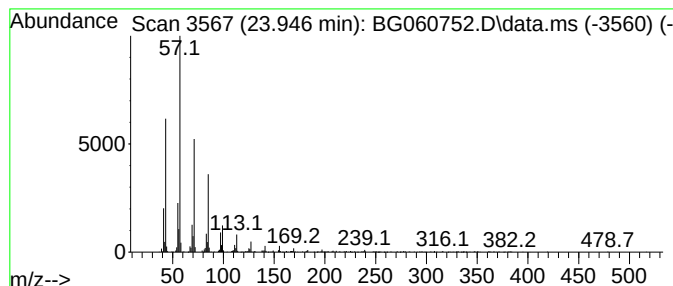
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.946	15.80 ng	992094	Perylene-d12	24.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	98
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	94
3			Octacosane	394	C28H58	000630-02-4	91
4			Hexacosane	366	C26H54	000630-01-3	90
5			Pentacosane	352	C25H52	000629-99-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040224\
Data File : BG060752.D
Acq On : 3 Apr 2024 00:50
Operator : MA/JU
Sample : P1879-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB-01(0-2)

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.176	22.8	ng	553444	1	7.953	484904	20.0
unknown3.687	3.687	3.7	ng	90130	1	7.953	484904	20.0
n-Hexadecanoic ...	18.241	12.0	ng	698494	4	17.330	1163600	20.0
Octadecanoic acid	19.516	3.1	ng	247710	5	21.596	1571740	20.0
Cycloeicosane	21.278	6.6	ng	521783	5	21.596	1571740	20.0
Oxalic acid, pe...	22.453	4.5	ng	356823	5	21.596	1571740	20.0
Heptacosane	23.946	15.8	ng	992094	6	24.733	1255570	20.0