

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
 Data File : BM049969.D
 Acq On : 18 Apr 2025 17:06
 Operator : RC/JU
 Sample : Q1828-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RT5417

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-BM040825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049969.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.887	318	323	336	rVB	1297790	1846029	10.42%	1.551%
2	5.357	396	403	425	rBV	6420281	9438459	53.27%	7.931%
3	5.963	501	506	513	rBV	198211	283017	1.60%	0.238%
4	6.951	666	674	689	rBV	5773954	9722392	54.87%	8.169%
5	7.769	804	813	821	rBV	1766039	2752479	15.53%	2.313%
6	8.928	1002	1010	1030	rBV	3690221	6269109	35.38%	5.268%
7	9.492	1100	1106	1120	rBV	104980	206360	1.16%	0.173%
8	10.563	1280	1288	1302	rBV	1844480	3220940	18.18%	2.706%
9	13.033	1699	1708	1725	rBV	9780263	14674939	82.82%	12.331%
10	14.410	1935	1942	1948	rBV	2669787	3786188	21.37%	3.181%
11	14.474	1948	1953	1961	rVB	460352	697611	3.94%	0.586%
12	14.810	2005	2010	2019	rBV	183471	299912	1.69%	0.252%
13	15.463	2116	2121	2128	rVB	218367	329935	1.86%	0.277%
14	15.768	2167	2173	2187	rBV	2067007	2902063	16.38%	2.439%
15	15.904	2189	2196	2215	rVV	7365668	10206983	57.60%	8.577%
16	16.110	2226	2231	2234	rBV	126445	210970	1.19%	0.177%
17	16.333	2264	2269	2278	rVB	263060	383966	2.17%	0.323%
18	16.821	2346	2352	2359	rBV2	258817	417899	2.36%	0.351%
19	17.157	2403	2409	2413	rBV	2868837	3986067	22.50%	3.349%
20	17.198	2413	2416	2421	rVB	984878	1264662	7.14%	1.063%
21	17.286	2427	2431	2437	rVB	512140	733045	4.14%	0.616%
22	18.057	2554	2562	2570	rBV2	1569214	2681965	15.14%	2.254%
23	18.227	2586	2591	2595	rBV3	196889	330958	1.87%	0.278%
24	19.215	2754	2759	2766	rBV	2215890	2834618	16.00%	2.382%
25	19.339	2776	2780	2789	rBV2	461353	836399	4.72%	0.703%
26	19.580	2812	2821	2829	rBV	1678638	2792889	15.76%	2.347%
27	19.780	2849	2855	2861	rBV	14876875	17719754	100.00%	14.889%
28	20.074	2902	2905	2912	rVB2	284656	423389	2.39%	0.356%
29	20.174	2919	2922	2926	rBV	185319	206838	1.17%	0.174%
30	21.074	3071	3075	3082	rBV3	605583	979913	5.53%	0.823%
31	21.392	3122	3129	3134	rBV2	3295984	6115677	34.51%	5.139%
32	21.439	3134	3137	3147	rVB	984655	1505853	8.50%	1.265%
33	22.503	3313	3318	3328	rVB	2105953	3311816	18.69%	2.783%
34	23.450	3474	3479	3485	rBV	614472	1457504	8.23%	1.225%
35	24.391	3633	3639	3648	rVB	1730310	4177984	23.58%	3.511%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049969.D
Acq On : 18 Apr 2025 17:06
Operator : RC/JU
Sample : Q1828-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT5417

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-BM040825.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

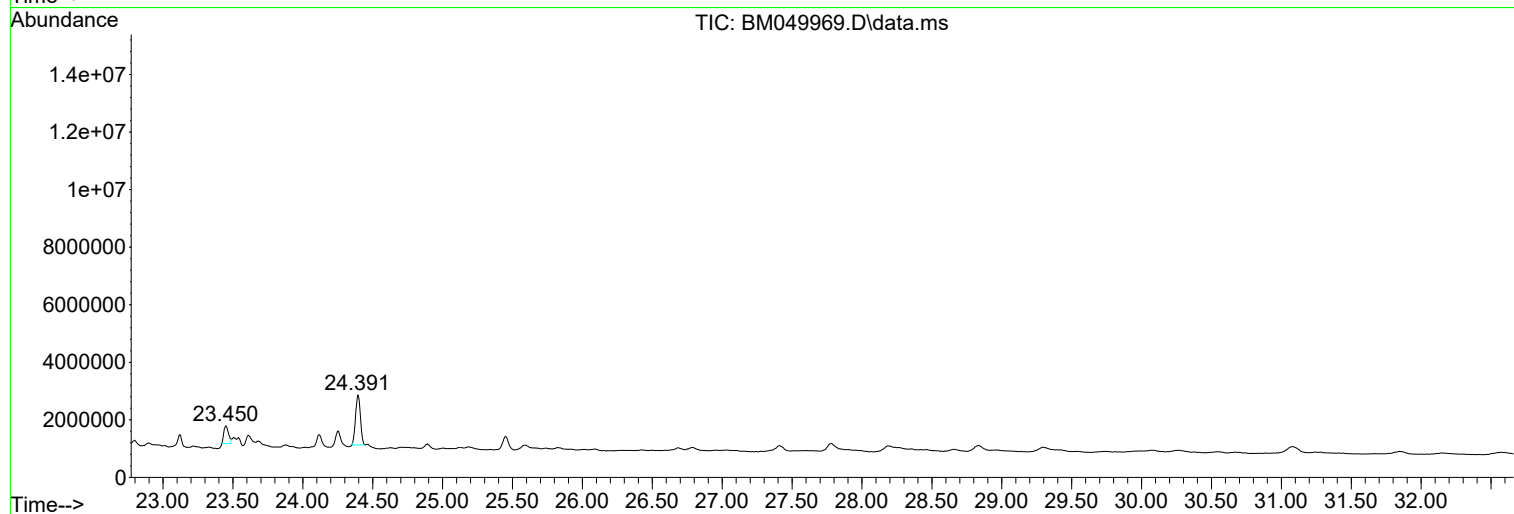
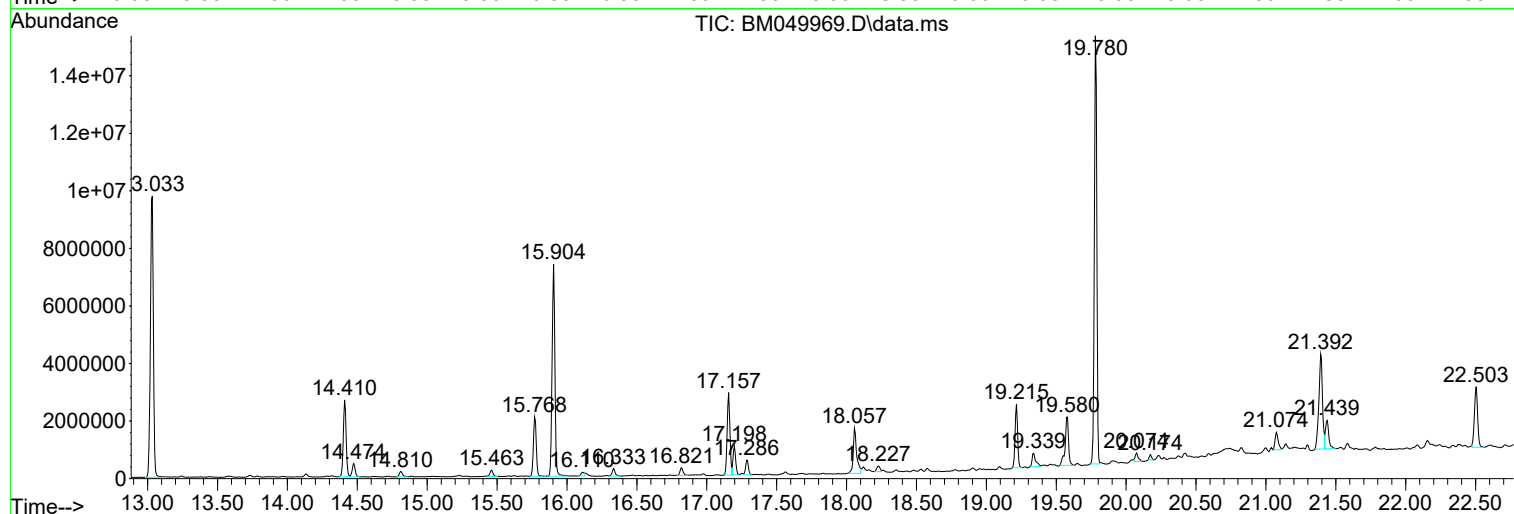
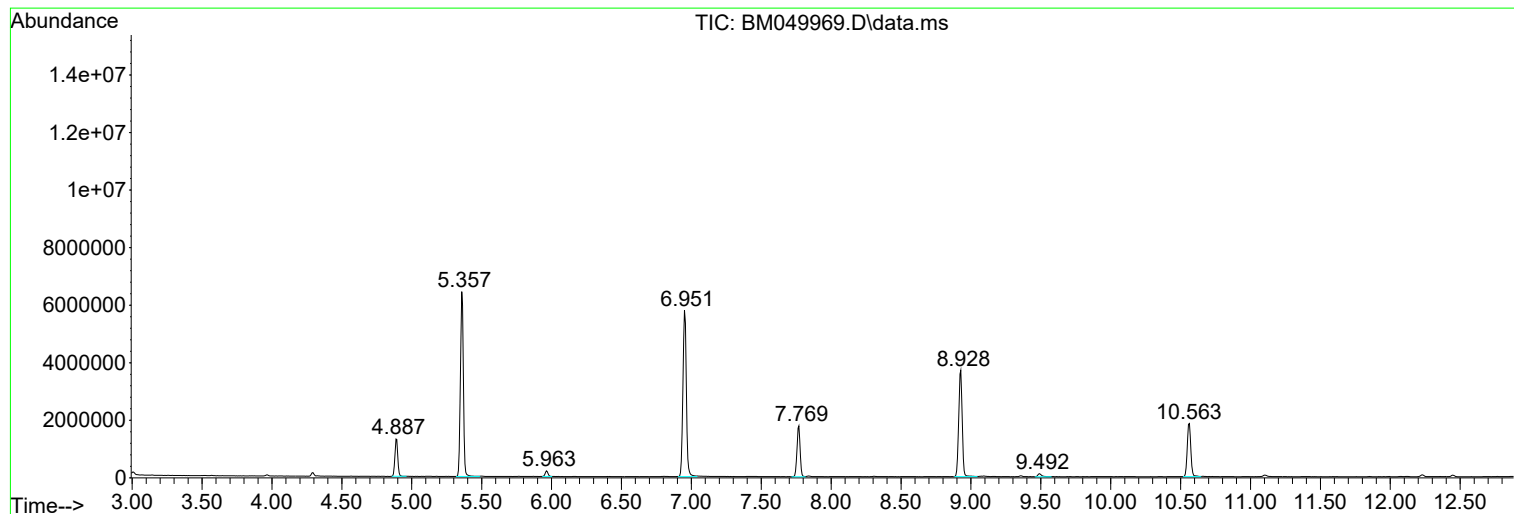
Sum of corrected areas: 119008582

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049969.D
Acq On : 18 Apr 2025 17:06
Operator : RC/JU
Sample : Q1828-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT5417

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.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_M\Data\BM041825\
Data File : BM049969.D
Acq On : 18 Apr 2025 17:06
Operator : RC/JU
Sample : Q1828-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT5417

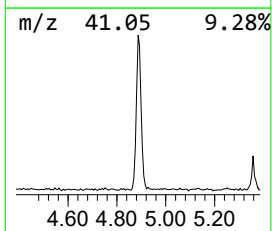
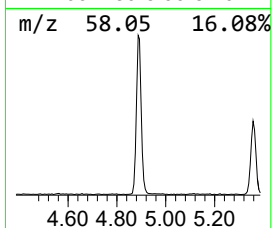
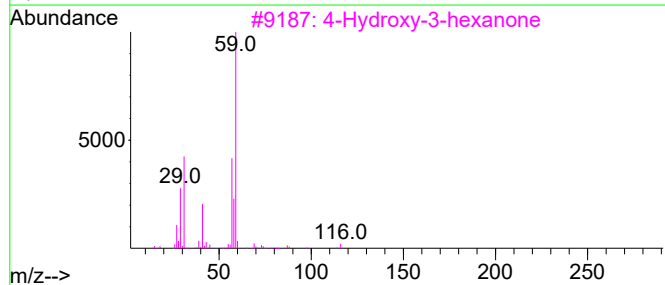
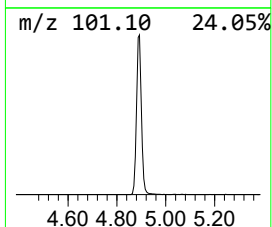
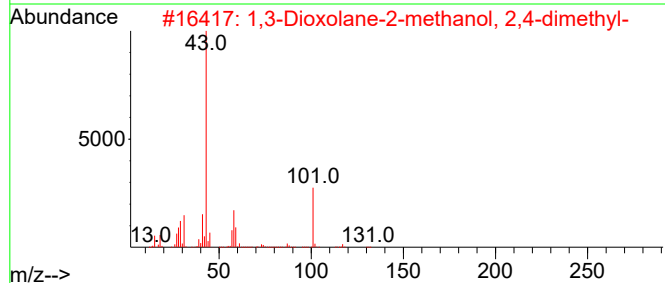
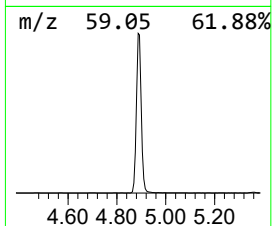
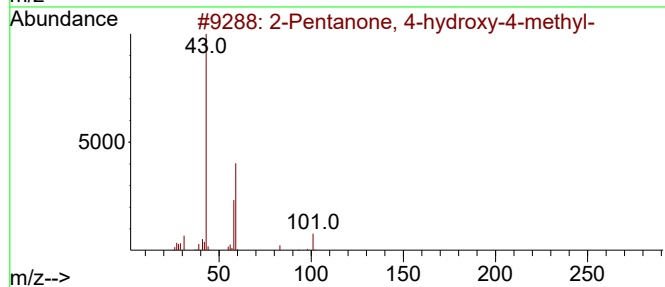
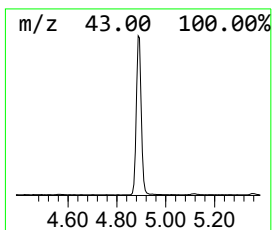
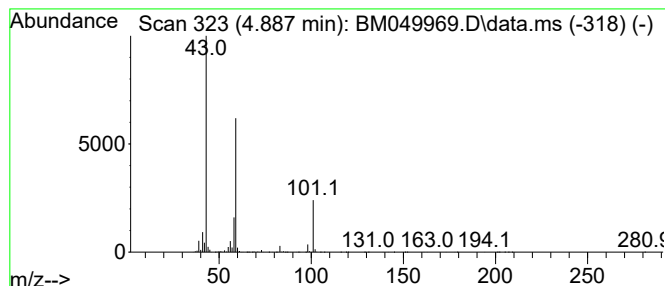
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.887	13.41 ng	1846030	1,4-Dichlorobenzene-d4	7.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25		
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049969.D
Acq On : 18 Apr 2025 17:06
Operator : RC/JU
Sample : Q1828-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT5417

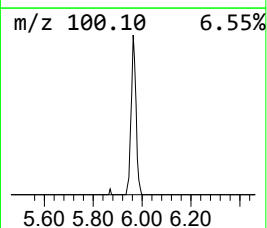
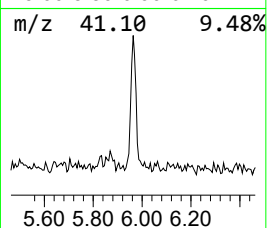
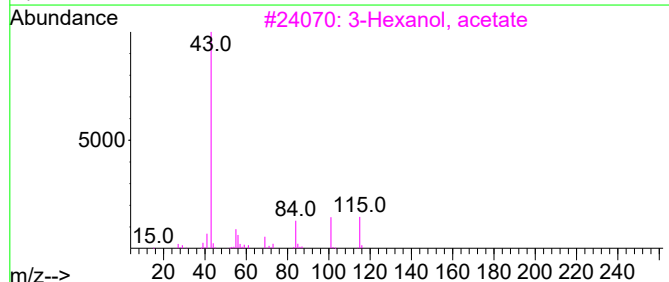
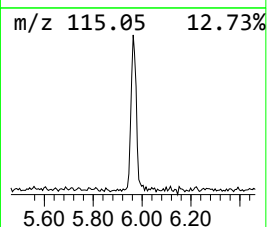
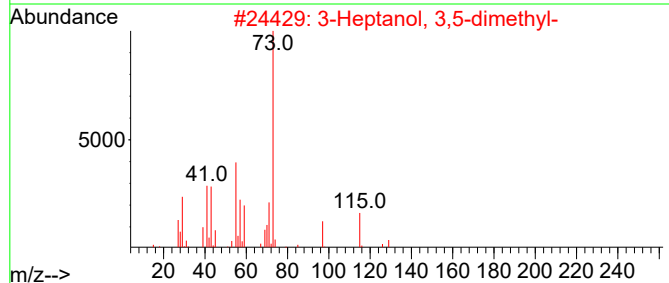
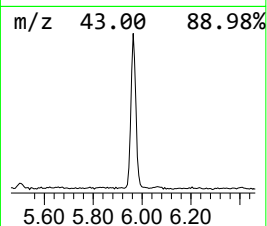
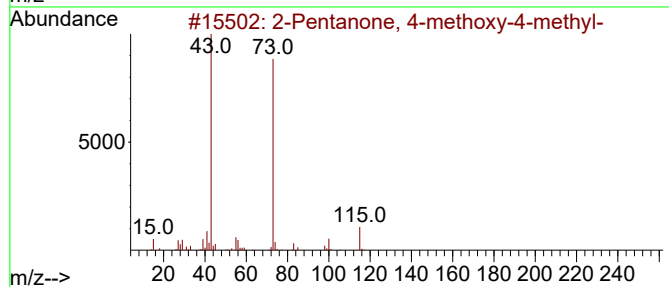
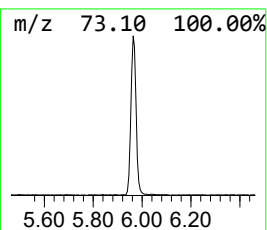
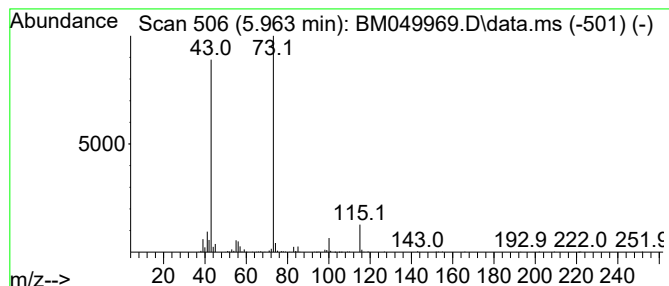
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.963	2.06 ng	283017	1,4-Dichlorobenzene-d4	7.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2			3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	25
3			3-Hexanol, acetate	144	C8H16O2	040780-64-1	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049969.D
Acq On : 18 Apr 2025 17:06
Operator : RC/JU
Sample : Q1828-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT5417

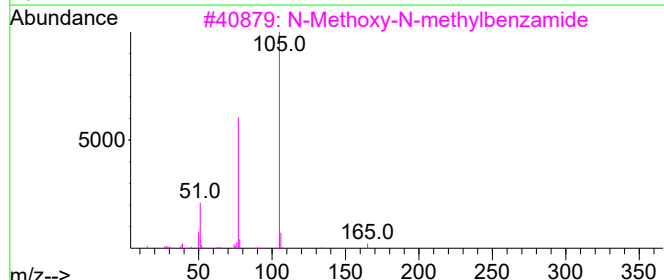
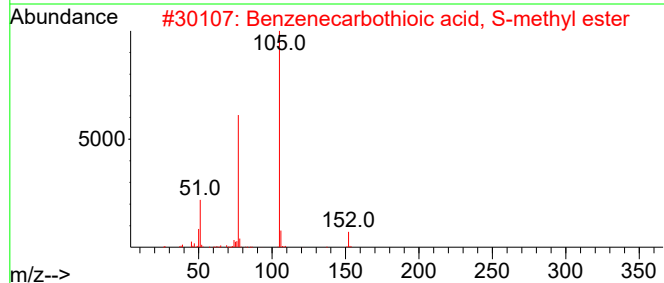
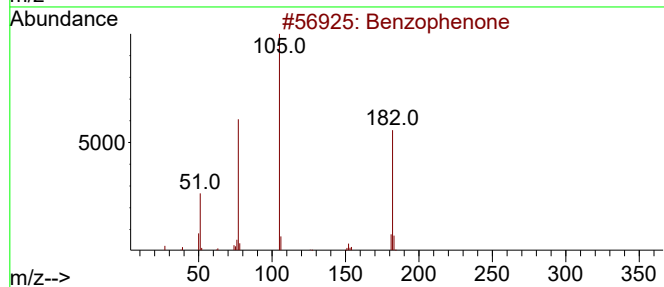
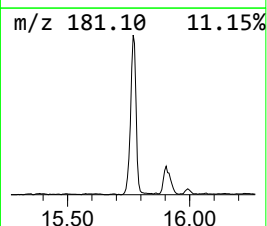
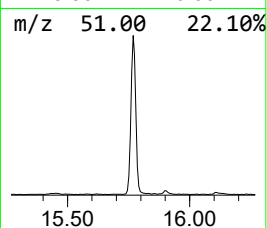
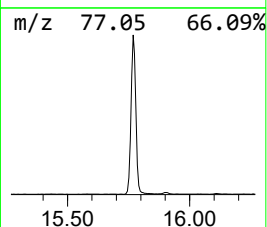
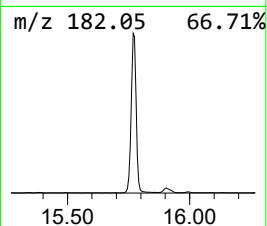
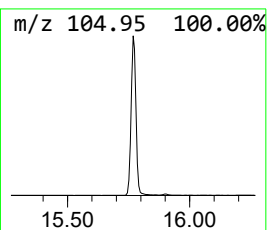
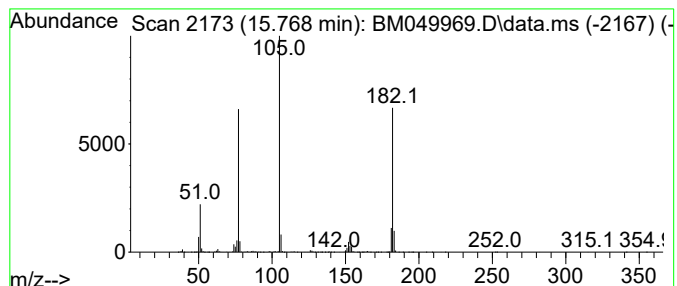
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.768	15.33 ng	2902060	Acenaphthene-d10	14.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	46
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	43
5			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049969.D
Acq On : 18 Apr 2025 17:06
Operator : RC/JU
Sample : Q1828-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT5417

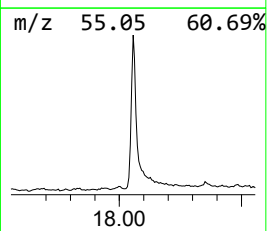
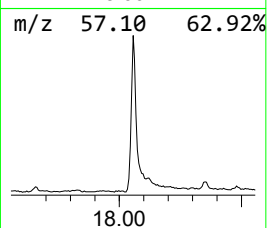
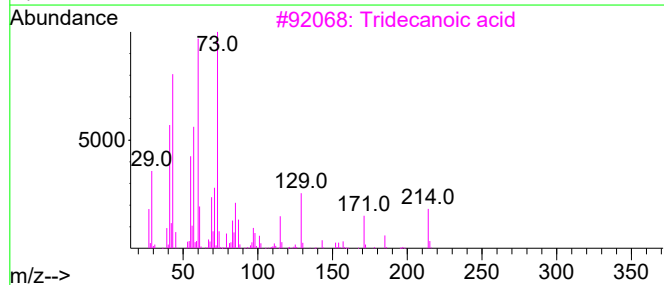
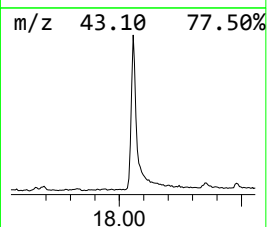
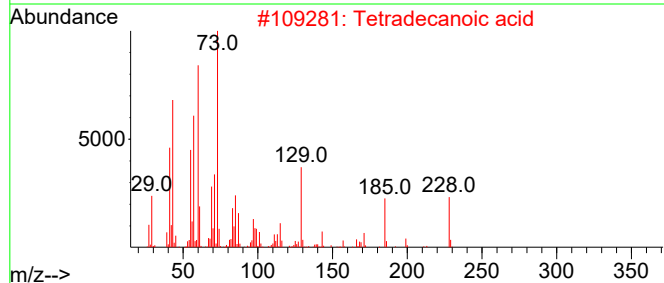
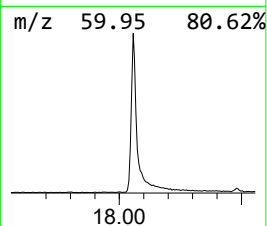
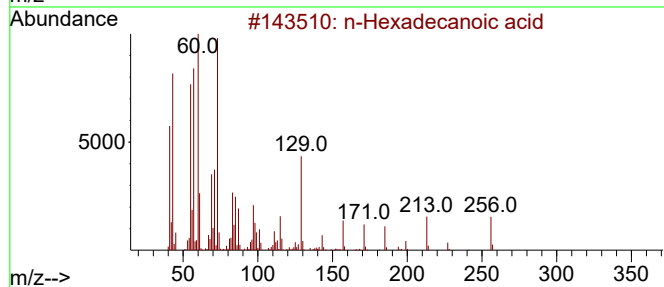
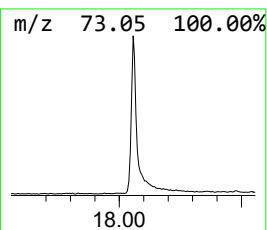
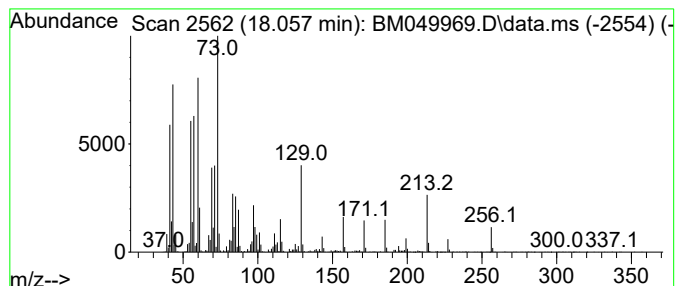
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.057	13.46 ng	2681970	Phenanthrene-d10	17.157

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	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Undecanoic acid	186	C11H22O2	000112-37-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049969.D
Acq On : 18 Apr 2025 17:06
Operator : RC/JU
Sample : Q1828-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT5417

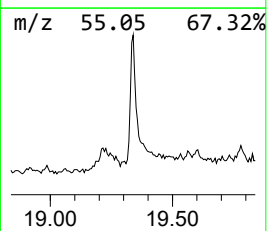
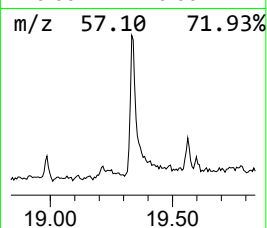
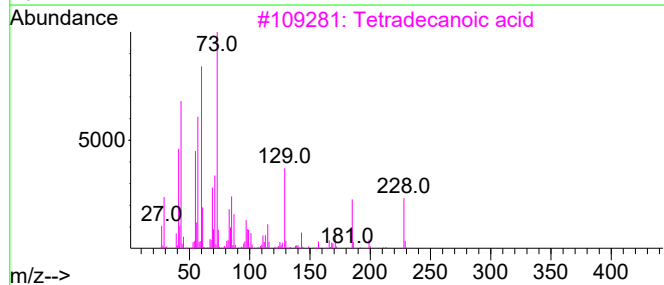
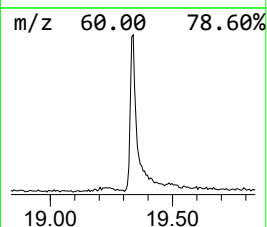
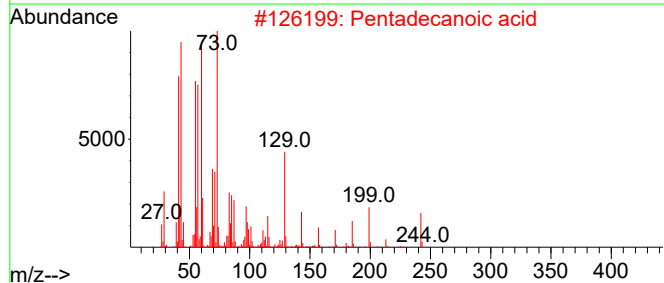
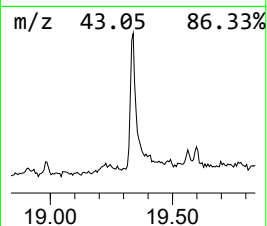
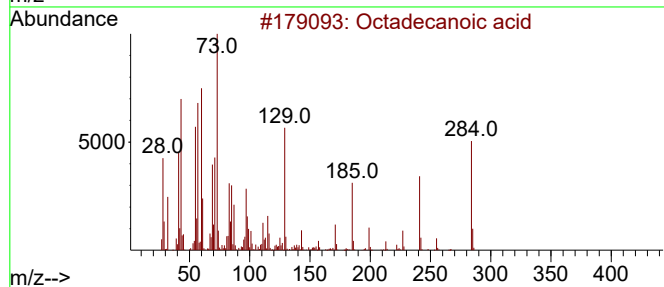
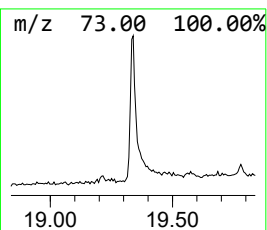
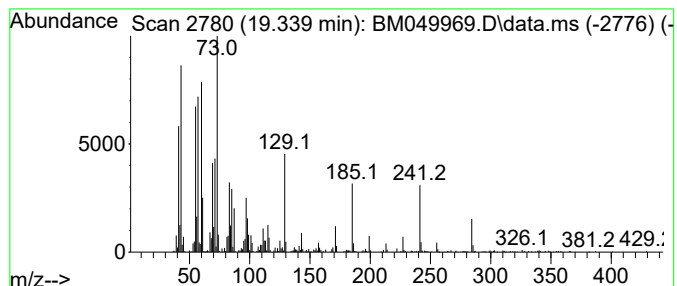
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.339	2.74 ng	836399	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049969.D
Acq On : 18 Apr 2025 17:06
Operator : RC/JU
Sample : Q1828-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT5417

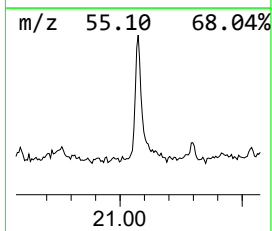
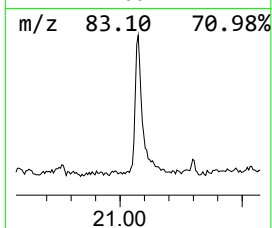
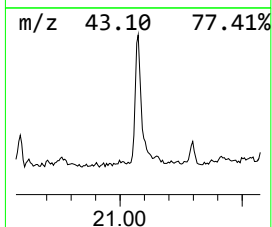
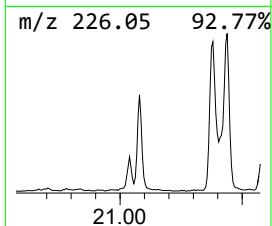
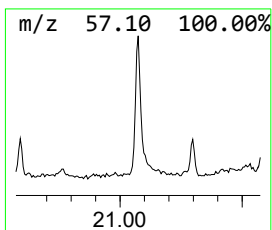
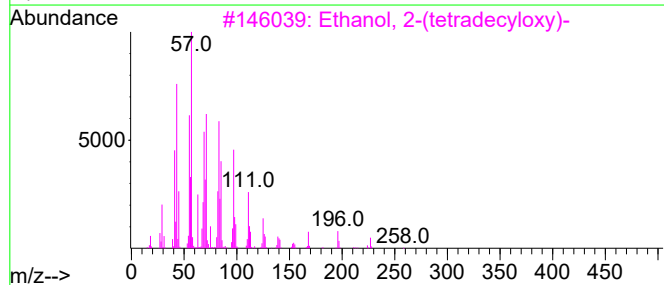
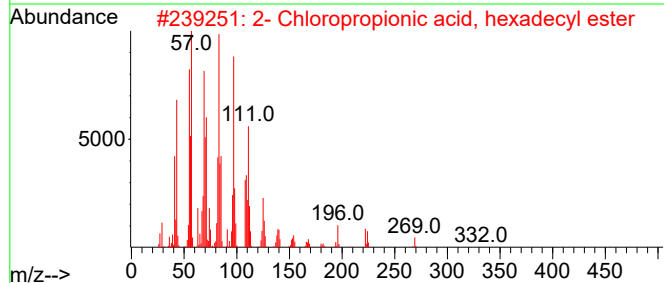
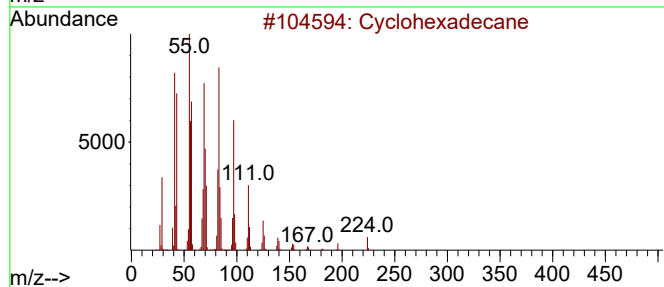
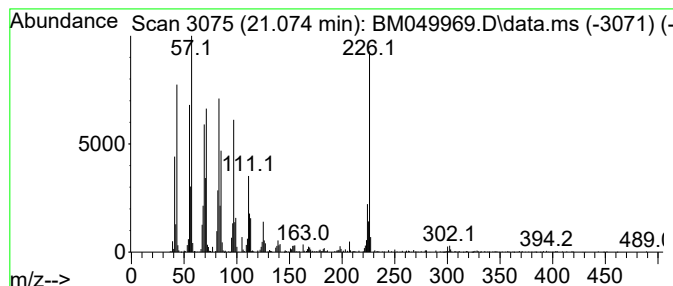
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	3.20 ng	979913	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	96
2			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	70
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	64
4			Trihexadecyl borate	735	C48H99B03	002665-11-4	64
5			1-Hexacosene	364	C26H52	018835-33-1	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049969.D
Acq On : 18 Apr 2025 17:06
Operator : RC/JU
Sample : Q1828-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT5417

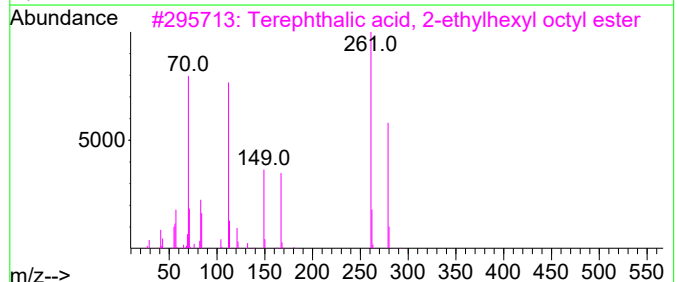
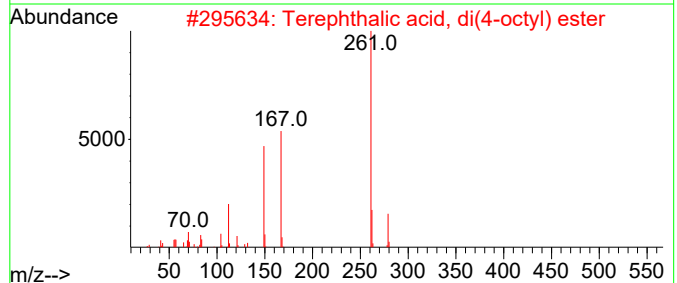
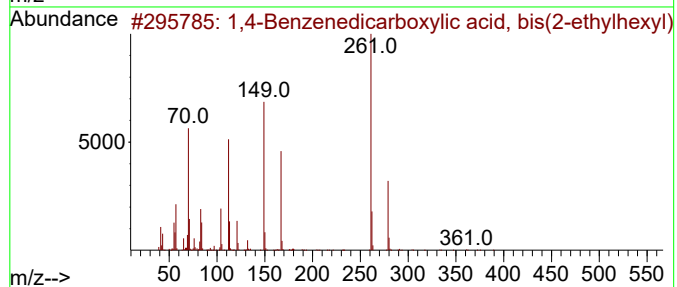
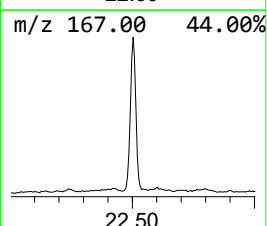
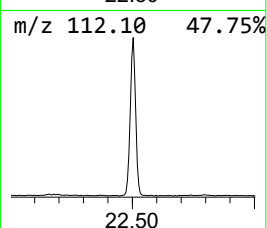
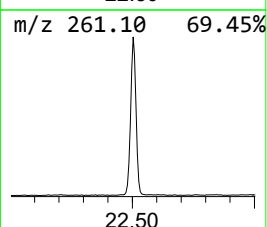
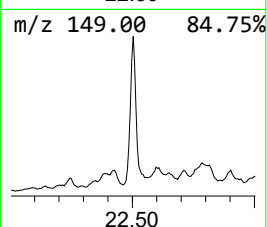
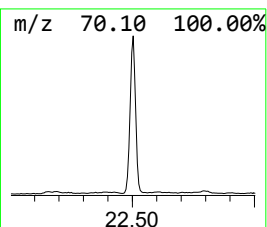
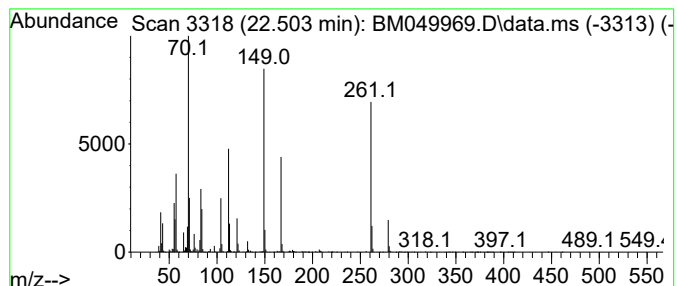
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.503	10.83 ng	3311820	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	76
2			Terephthalic acid, di(4-octyl) e...	390	C24H3804	1000323-74-2	50
3			Terephthalic acid, 2-ethylhexyl ...	390	C24H3804	1000324-00-5	46
4			1,3-Benzenedicarboxylic acid, bi...	390	C24H3804	000137-89-3	46
5			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049969.D
Acq On : 18 Apr 2025 17:06
Operator : RC/JU
Sample : Q1828-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT5417

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.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
2-Pentanone, 4-...	4.887	13.4	ng	1846030	1	7.769	2752480	20.0
2-Pentanone, 4-...	5.963	2.1	ng	283017	1	7.769	2752480	20.0
Benzophenone	15.768	15.3	ng	2902060	3	14.410	3786190	20.0
n-Hexadecanoic ...	18.057	13.5	ng	2681970	4	17.157	3986070	20.0
Octadecanoic acid	19.339	2.7	ng	836399	5	21.392	6115680	20.0
Cyclohexadecane	21.074	3.2	ng	979913	5	21.392	6115680	20.0
1,4-Benzenedica...	22.503	10.8	ng	3311820	5	21.392	6115680	20.0