

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
 Data File : BG060766.D
 Acq On : 3 Apr 2024 17:31
 Operator : MA/JU
 Sample : P1955-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CHRT-20103

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: BG060766.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.099	13	19	27	rBV	147425	350996	12.93%	1.616%
2	3.175	27	32	50	rVB	610976	1090116	40.16%	5.020%
3	3.686	116	119	125	rBV	29356	44226	1.63%	0.204%
4	5.537	426	434	446	rBV	1077798	1737860	64.03%	8.002%
5	7.118	695	703	711	rBV	1147293	1908199	70.30%	8.787%
6	7.958	837	846	852	rBV	283372	477481	17.59%	2.199%
7	9.110	1034	1042	1050	rBV	674779	1162204	42.82%	5.352%
8	10.531	1277	1284	1290	rBV	119040	195023	7.18%	0.898%
9	10.755	1313	1322	1329	rBV	378859	675613	24.89%	3.111%
10	11.489	1438	1447	1452	rBV5	14601	33513	1.23%	0.154%
11	13.211	1733	1740	1748	rBV	1263872	1967467	72.48%	9.060%
12	13.381	1761	1769	1776	rBV8	47341	114124	4.20%	0.526%
13	13.945	1862	1865	1873	rVB5	40325	72553	2.67%	0.334%
14	14.021	1873	1878	1883	rBV2	91643	161058	5.93%	0.742%
15	14.092	1887	1890	1894	rVV3	46469	61665	2.27%	0.284%
16	14.139	1895	1898	1902	rVB5	28407	43683	1.61%	0.201%
17	14.251	1914	1917	1922	rVB4	31846	44893	1.65%	0.207%
18	14.339	1928	1932	1937	rBV8	56106	121088	4.46%	0.558%
19	14.427	1944	1947	1955	rVB	139417	218054	8.03%	1.004%
20	14.503	1956	1960	1965	rBV5	49138	85445	3.15%	0.393%
21	14.585	1966	1974	1985	rVV	636007	1200495	44.23%	5.528%
22	15.132	2063	2067	2074	rBV6	73711	157525	5.80%	0.725%
23	15.390	2106	2111	2116	rBV	228181	354943	13.08%	1.634%
24	16.072	2222	2227	2233	rBV	1417583	2129220	78.44%	9.804%
25	16.354	2271	2275	2284	rVB	387268	563680	20.77%	2.596%
26	17.177	2412	2415	2422	rVB	366254	541826	19.96%	2.495%
27	17.335	2438	2442	2446	rBV	684018	946949	34.89%	4.360%
28	19.962	2885	2889	2895	rVB	2088977	2714311	100.00%	12.499%
29	21.601	3163	3168	3174	rVB	774319	1203472	44.34%	5.542%
30	24.744	3695	3703	3712	rVB	474001	1339098	49.33%	6.166%

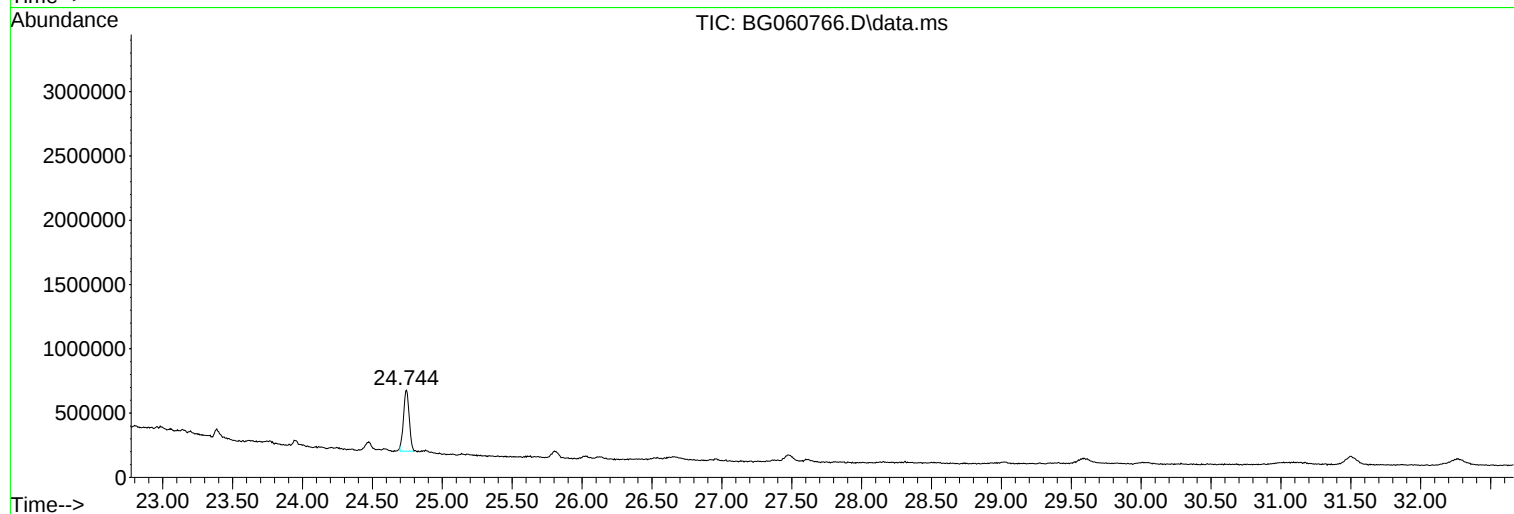
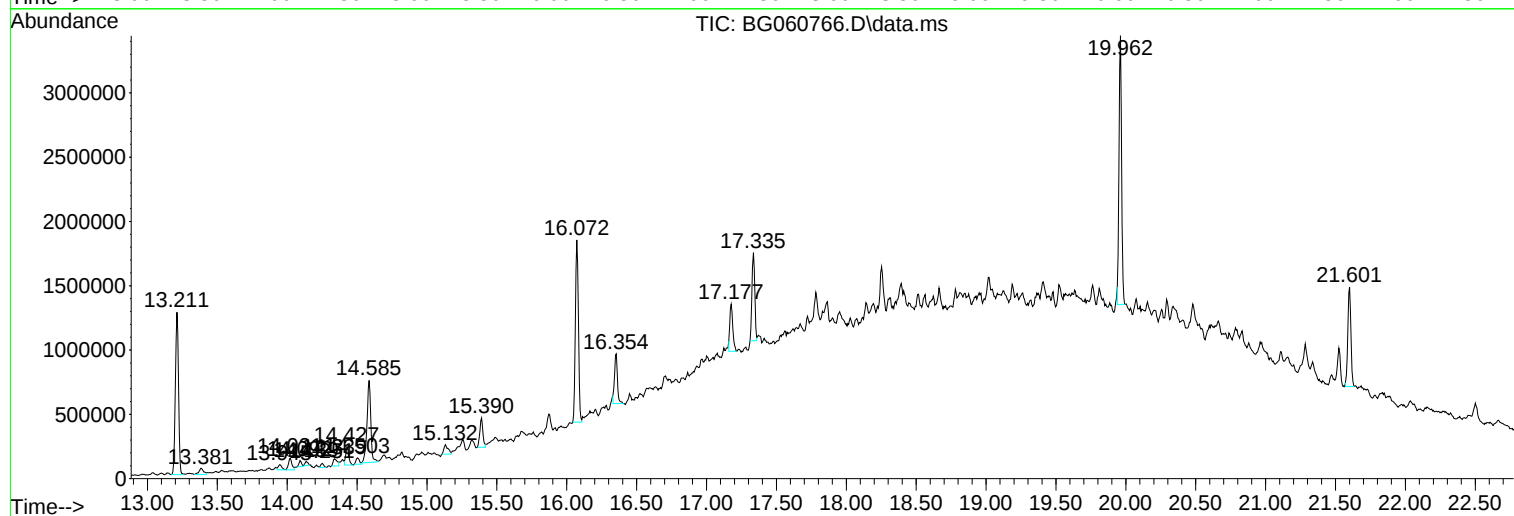
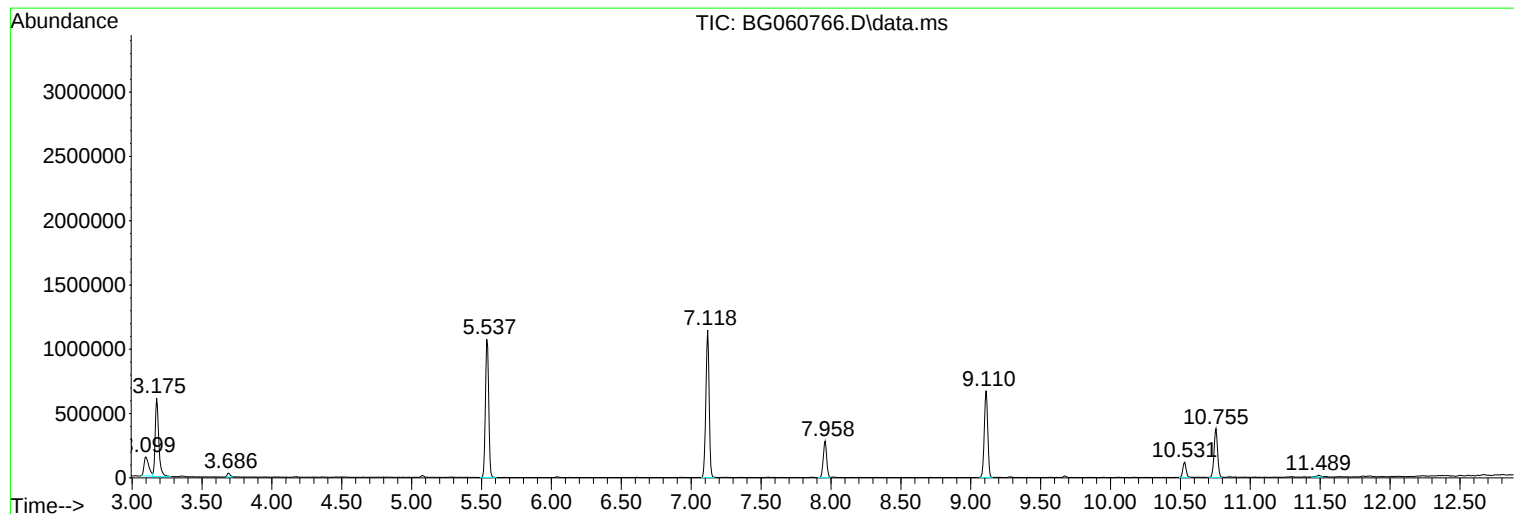
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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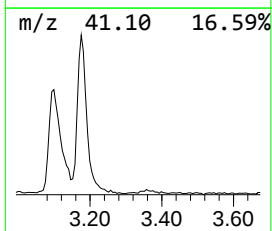
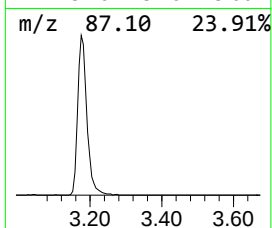
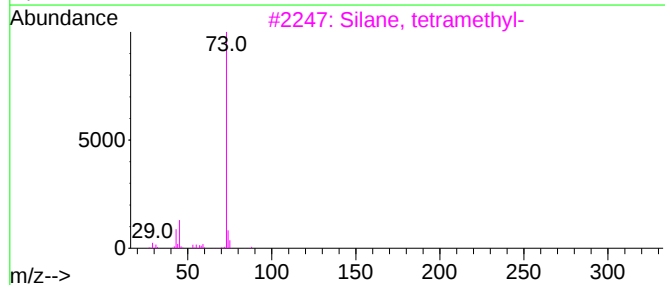
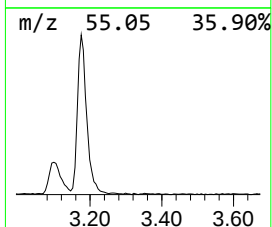
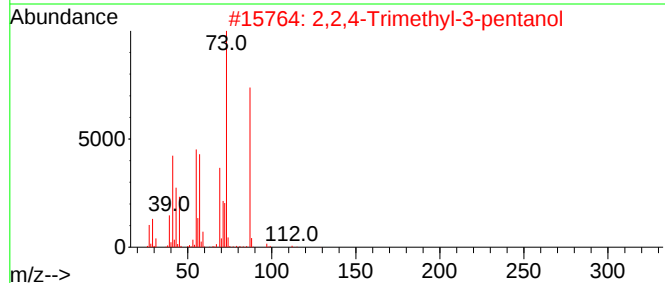
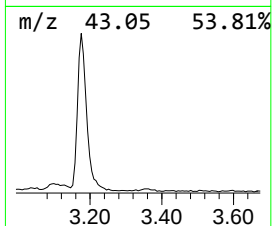
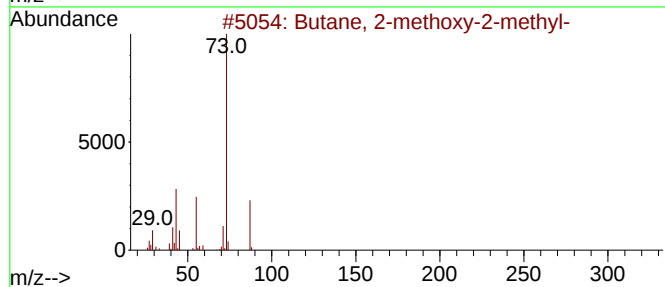
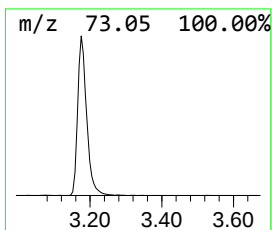
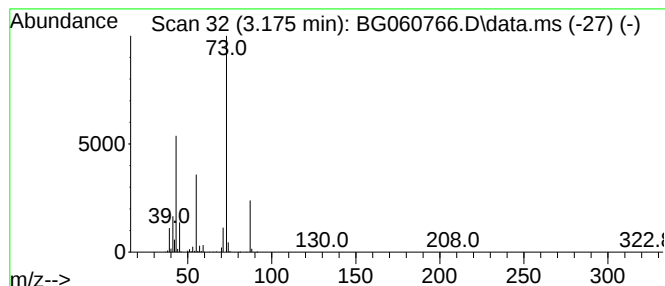
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.175	45.66 ng	1090120	1,4-Dichlorobenzene-d4	7.958

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	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4			Acetic acid, (acetyloxy)-	118	C4H6O4	013831-30-6	12
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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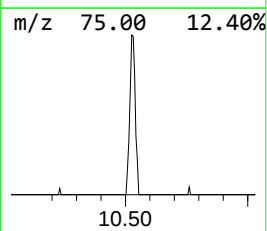
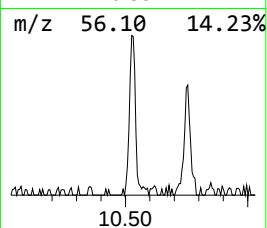
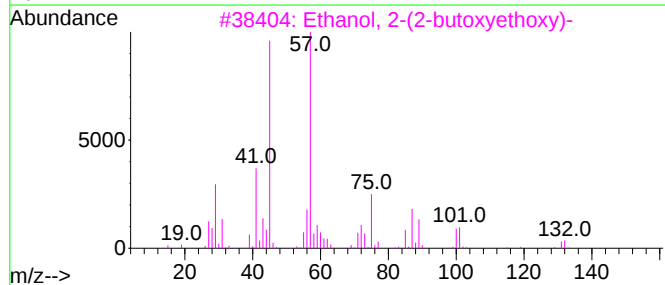
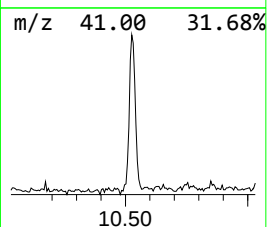
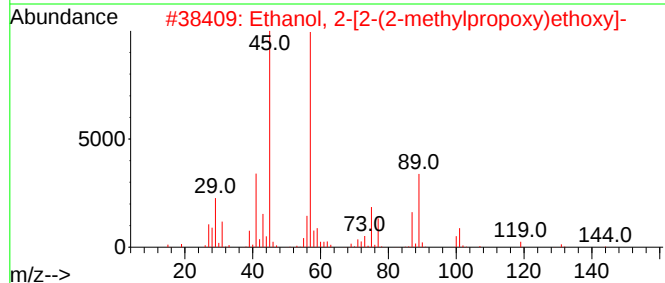
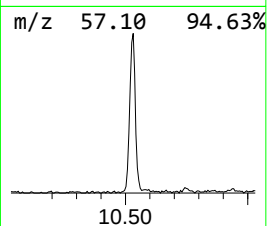
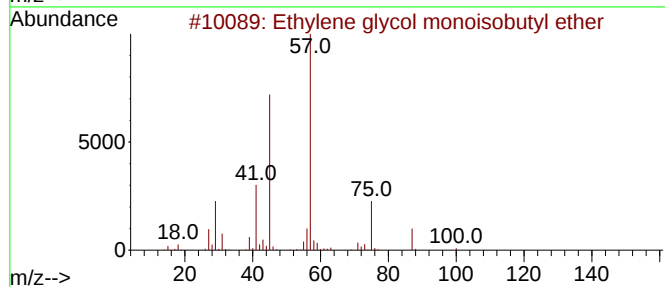
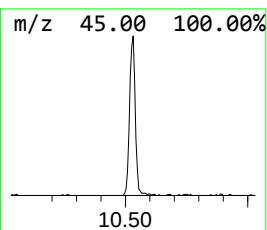
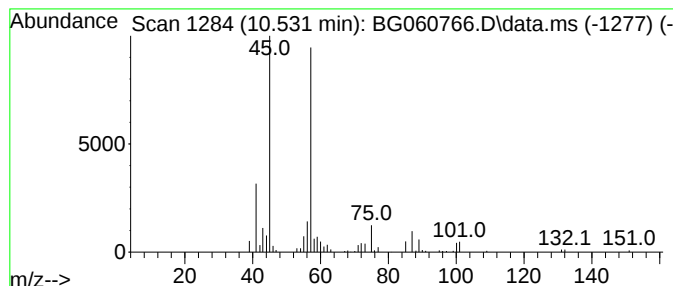
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Ethylene glycol monoisobuty... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.531	5.77 ng	195023	Naphthalene-d8	10.755

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
3			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	47
4			1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	47
5			Butyl lactate	146	C7H14O3	000138-22-7	47



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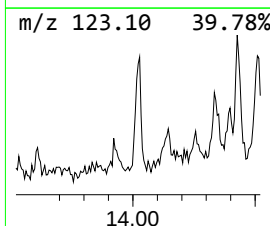
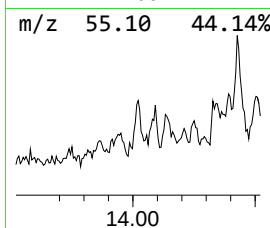
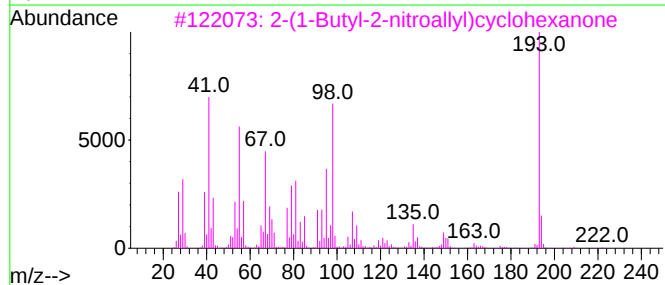
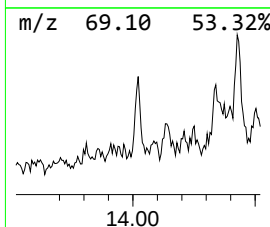
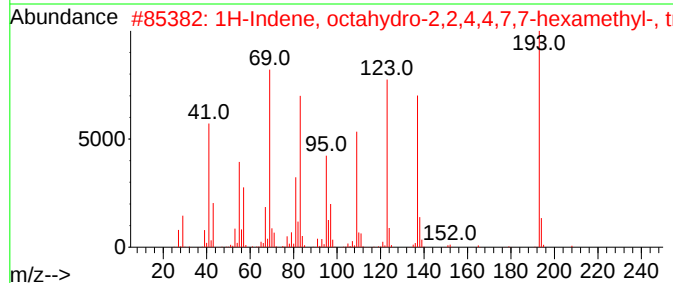
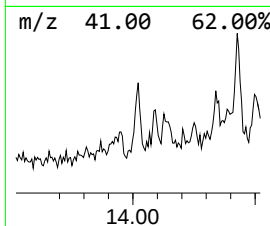
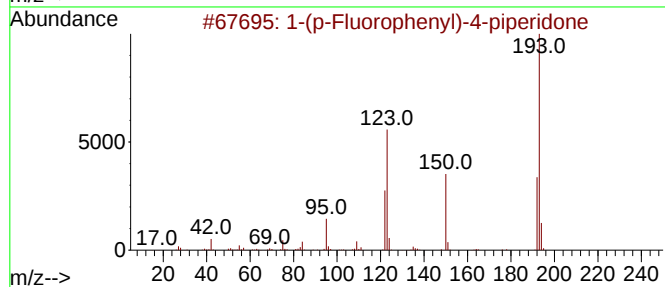
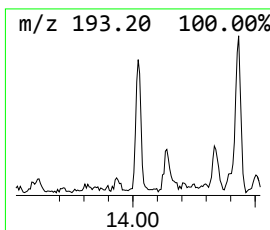
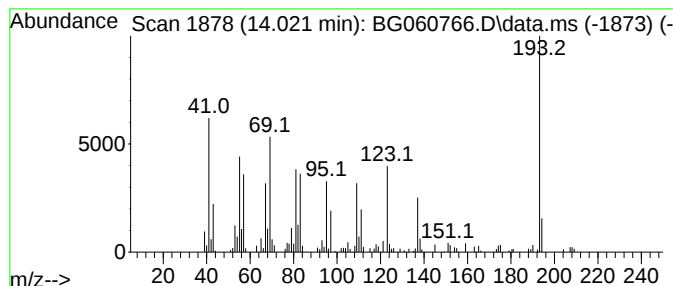
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown14.021 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.021	2.68 ng	161058	Acenaphthene-d10	14.586

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	43
2		1H-Indene, octahydro-2,2,4,7,7...	208	C15H28	054832-83-6	38
3		2-(1-Butyl-2-nitroallyl)cyclohex...	239	C13H21NO3	1000192-05-9	32
4		2-Anthracenamine	193	C14H11N	000613-13-8	30
5		2(1H)-Naphthalenone, octahydro-4...	194	C13H22O	007056-56-6	27



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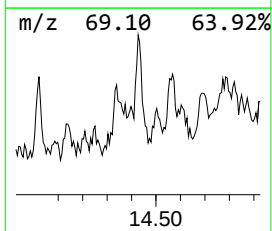
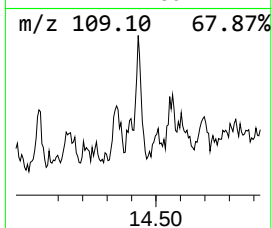
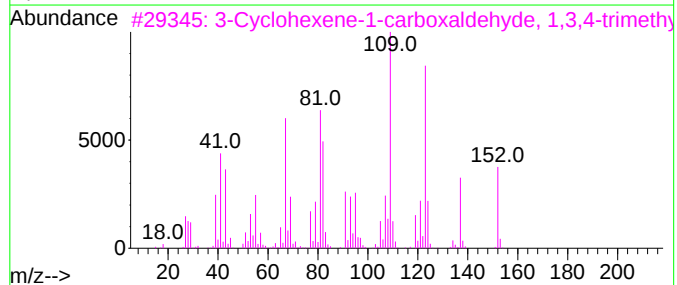
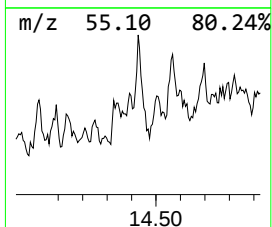
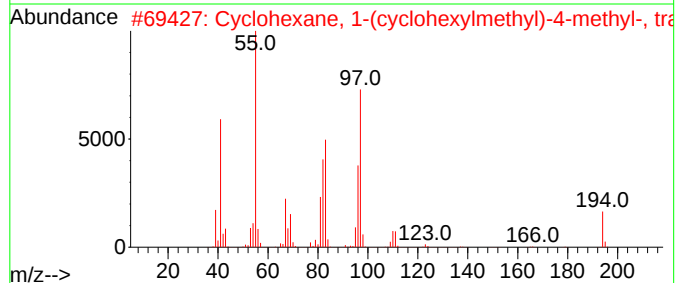
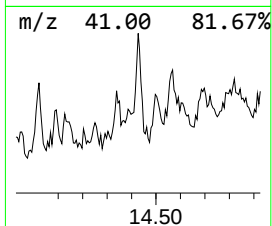
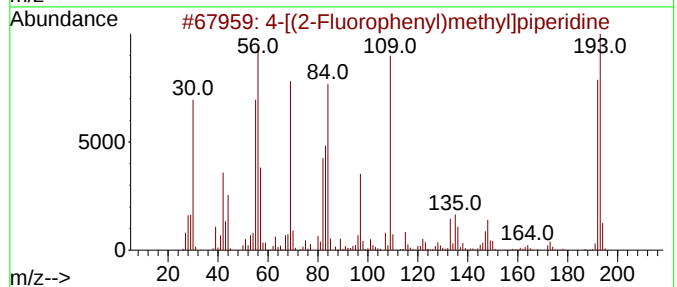
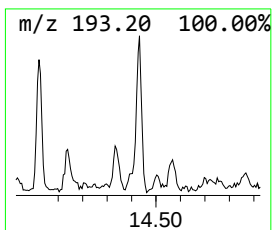
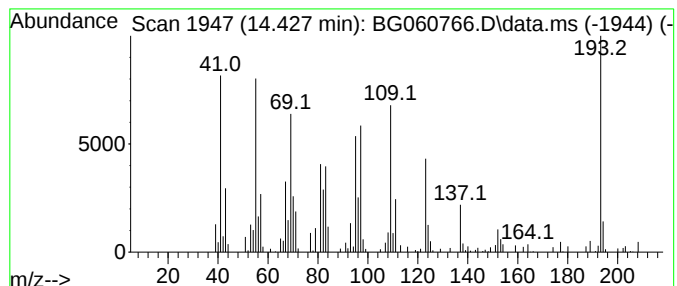
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 unknown14.427 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.427	3.63 ng	218054	Acenaphthene-d10	14.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-[(2-Fluorophenyl)methyl]piperi...	193	C12H16FN	194288-97-6	46		
2	Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26	054823-98-2	38		
3	3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	25		
4	Cyclopentane, 2-isopropyl-1,3-di...	140	C10H20	032281-85-9	25		
5	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004795-86-2	20		



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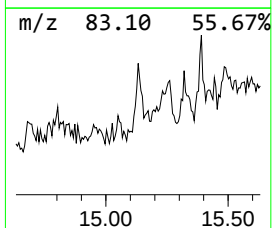
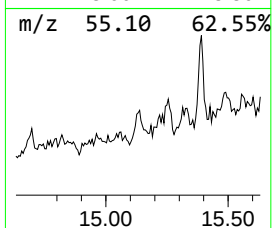
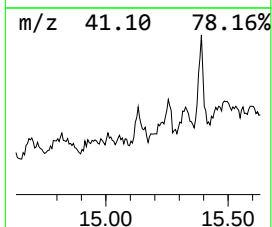
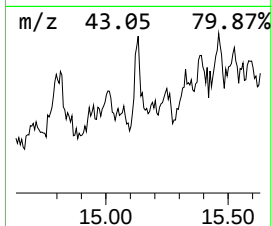
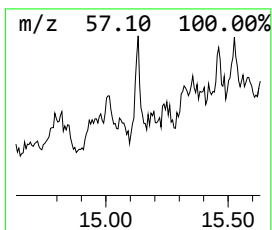
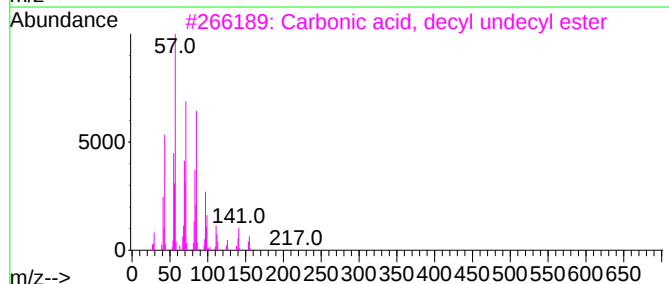
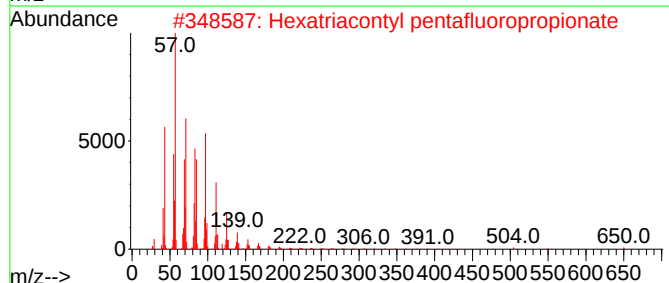
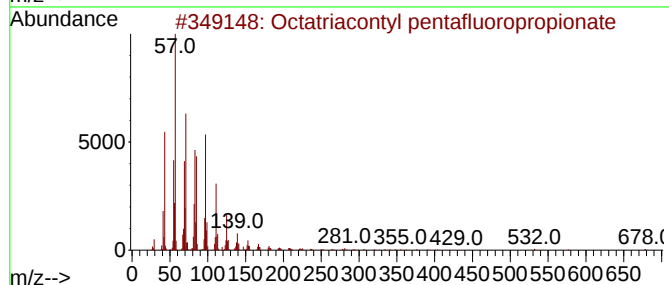
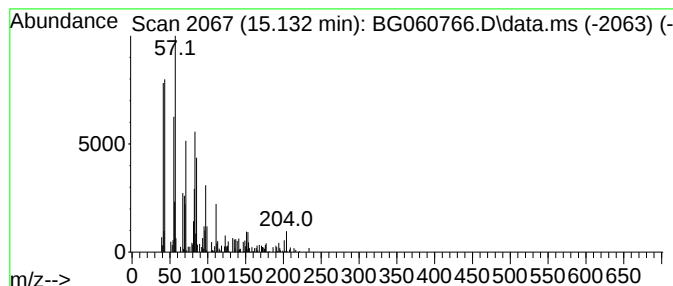
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Peak Number 7 Octatriacontyl pentafluorop... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.132	2.62 ng	157525	Acenaphthene-d10	14.586	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	52
2	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	50
3	Carbonic acid, decyl undecyl ester	356	C22H44O3	1000383-16-0	47
4	Propyl triacontyl ether	481	C33H68O	1000406-28-6	46
5	Octacosyl propyl ether	452	C31H64O	1000406-28-5	46



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CHRT-20103

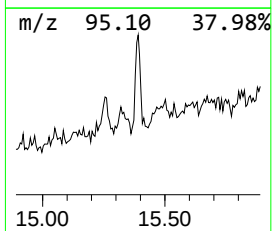
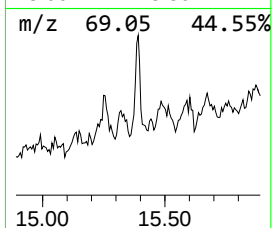
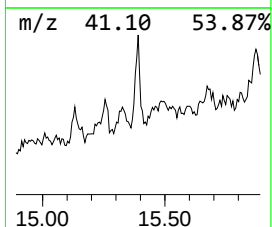
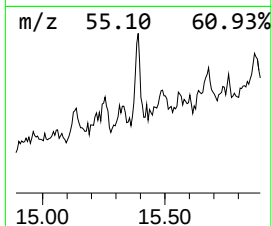
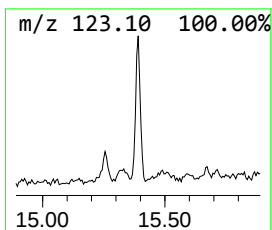
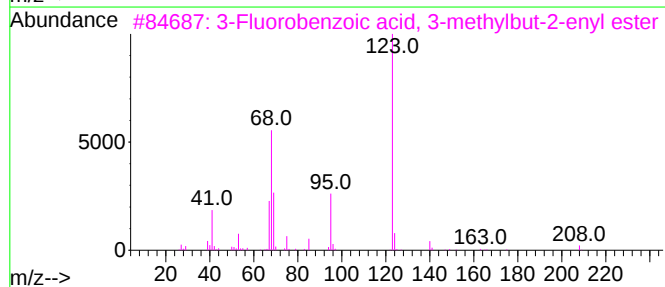
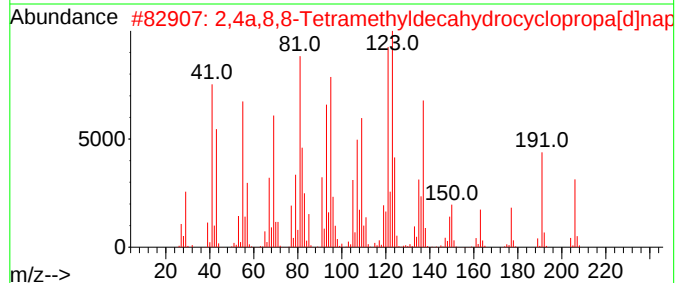
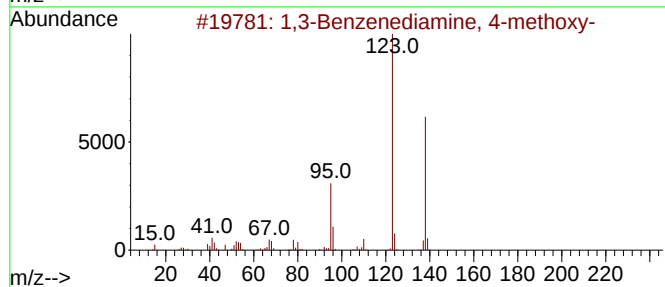
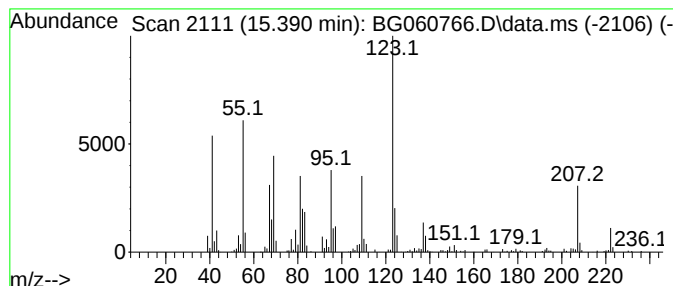
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.390 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.390	5.91 ng	354943	Acenaphthene-d10	14.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	46
2			2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	45
3			3-Fluorobenzoic acid, 3-methylbu...	208	C12H13F02	154559-38-3	43
4			Magnesium, bis(2,4-pentanedionat...	222	C10H14MgO4	014024-56-7	40
5			2-Fluorobenzoic acid, 4-tridecyl...	322	C20H31F02	1000280-61-2	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
Data File : BG060766.D
Acq On : 3 Apr 2024 17:31
Operator : MA/JU
Sample : P1955-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-20103

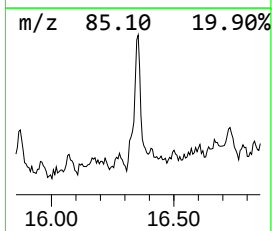
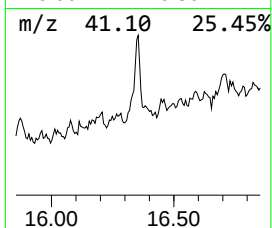
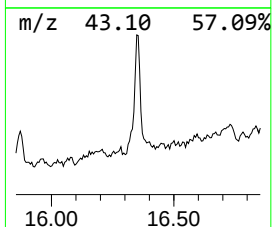
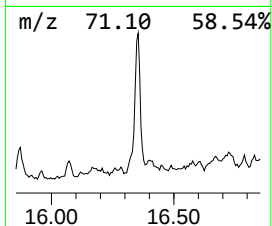
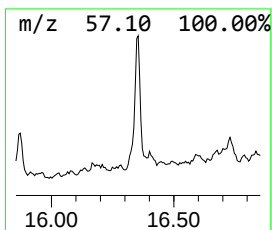
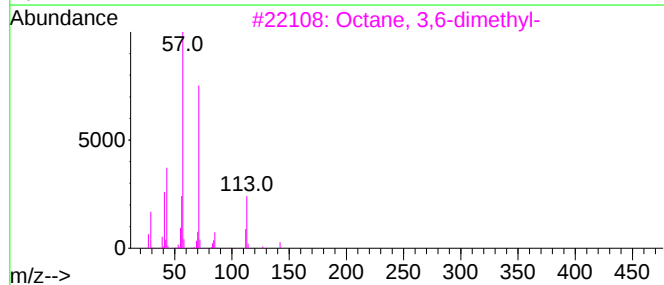
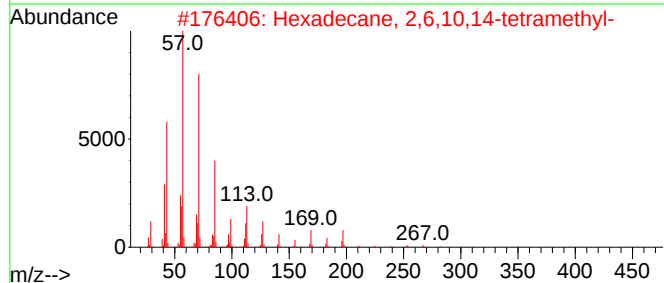
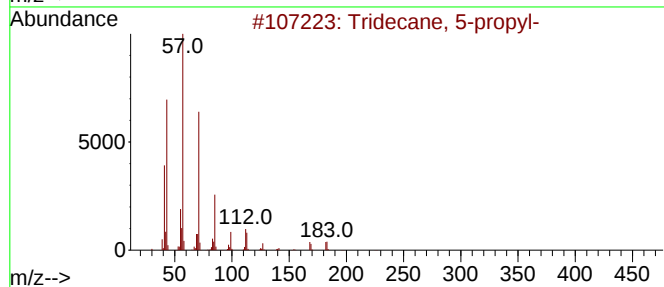
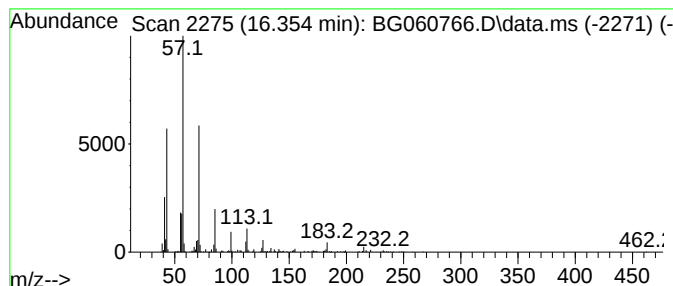
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tridecane, 5-propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.354	11.91 ng	563680	Phenanthrene-d10	17.335

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 5-propyl-	226	C16H34	055045-11-9	87
2			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	78
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	70
4			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	59
5			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
Data File : BG060766.D
Acq On : 3 Apr 2024 17:31
Operator : MA/JU
Sample : P1955-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-20103

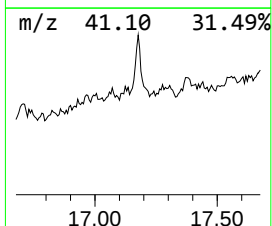
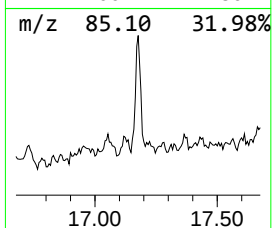
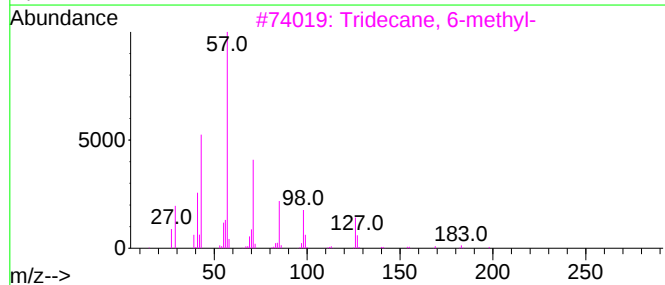
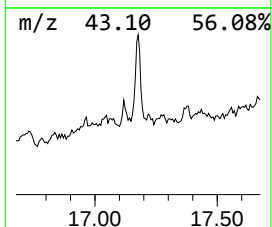
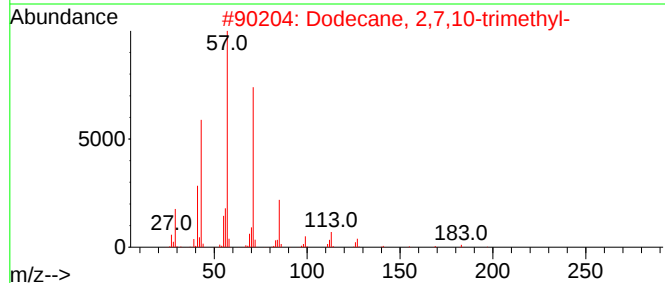
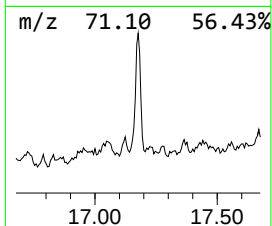
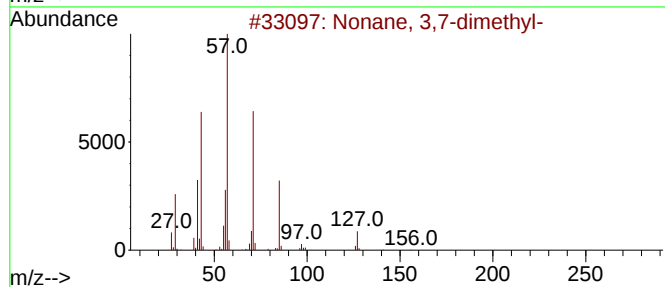
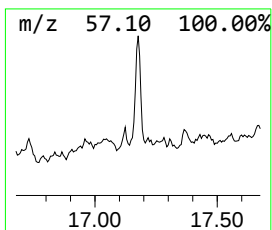
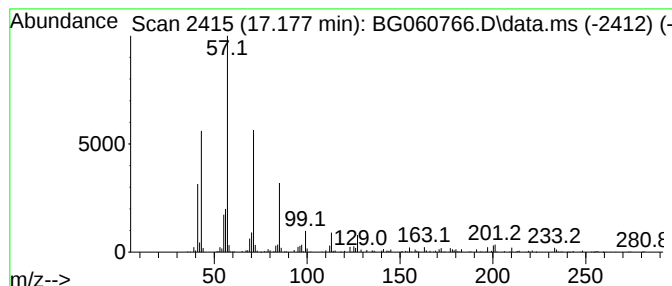
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonane, 3,7-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.177	11.44 ng	541826	Phenanthrene-d10	17.335

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	76
2			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
3			Tridecane, 6-methyl-	198	C14H30	013287-21-3	59
4			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	58
5			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
Data File : BG060766.D
Acq On : 3 Apr 2024 17:31
Operator : MA/JU
Sample : P1955-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-20103

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
Butane, 2-metho...	3.175	45.7	ng	1090120	1	7.958	477481	20.0
Ethylene glycol...	10.531	5.8	ng	195023	2	10.755	675613	20.0
unknown14.021	14.021	2.7	ng	161058	3	14.586	1200500	20.0
unknown14.339	14.339	2.0	ng	121088	3	14.586	1200500	20.0
unknown14.427	14.427	3.6	ng	218054	3	14.586	1200500	20.0
Octatriacontyl ...	15.132	2.6	ng	157525	3	14.586	1200500	20.0
unknown15.390	15.390	5.9	ng	354943	3	14.586	1200500	20.0
Tridecane, 5-pr...	16.354	11.9	ng	563680	4	17.335	946949	20.0
Nonane, 3,7-dim...	17.177	11.4	ng	541826	4	17.335	946949	20.0