

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
 Data File : BP016461.D
 Acq On : 01 Aug 2023 17:54
 Operator : MA/JU
 Sample : 03715-09
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 T842-CT-01

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_P\Methods\8270E-BP072723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP016461.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.593	385	392	400	rBV	8260207	12043894	33.59%	7.002%
2	7.216	660	668	686	rBV	7775094	13056204	36.41%	7.591%
3	8.081	808	815	829	rBV	1907912	3116723	8.69%	1.812%
4	8.328	850	857	868	rBV	340640	561071	1.56%	0.326%
5	9.275	1008	1018	1031	rBV	4952799	8213865	22.91%	4.776%
6	10.910	1288	1296	1305	rBV	2678533	4545655	12.68%	2.643%
7	13.351	1700	1711	1722	rBV	12401616	18336792	51.14%	10.661%
8	14.180	1847	1852	1862	rVB	691068	956998	2.67%	0.556%
9	14.339	1873	1879	1891	rBV	527422	804658	2.24%	0.468%
10	14.727	1936	1945	1952	rVB	3760261	5538112	15.45%	3.220%
11	16.104	2171	2179	2185	rBV	22260457	35856942	100.00%	20.847%
12	16.227	2193	2200	2214	rBV	7969201	12125400	33.82%	7.050%
13	17.492	2408	2415	2426	rBV	4198486	6154128	17.16%	3.578%
14	18.339	2553	2559	2571	rBV	2891895	4198934	11.71%	2.441%
15	19.574	2765	2769	2790	rVB	1867923	2648602	7.39%	1.540%
16	19.862	2813	2818	2821	rBV	674298	884781	2.47%	0.514%
17	19.898	2821	2824	2838	rVB	1428912	2016429	5.62%	1.172%
18	20.039	2842	2848	2854	rBV	16672401	21077884	58.78%	12.255%
19	21.127	3029	3033	3039	rBV3	272032	390985	1.09%	0.227%
20	21.251	3050	3054	3064	rBV	1017084	1375524	3.84%	0.800%
21	21.592	3106	3112	3118	rVB	3409495	4530415	12.63%	2.634%
22	24.192	3547	3554	3569	rVB	1834311	4121954	11.50%	2.396%
23	24.703	3632	3641	3655	rVB	4095504	9443290	26.34%	5.490%

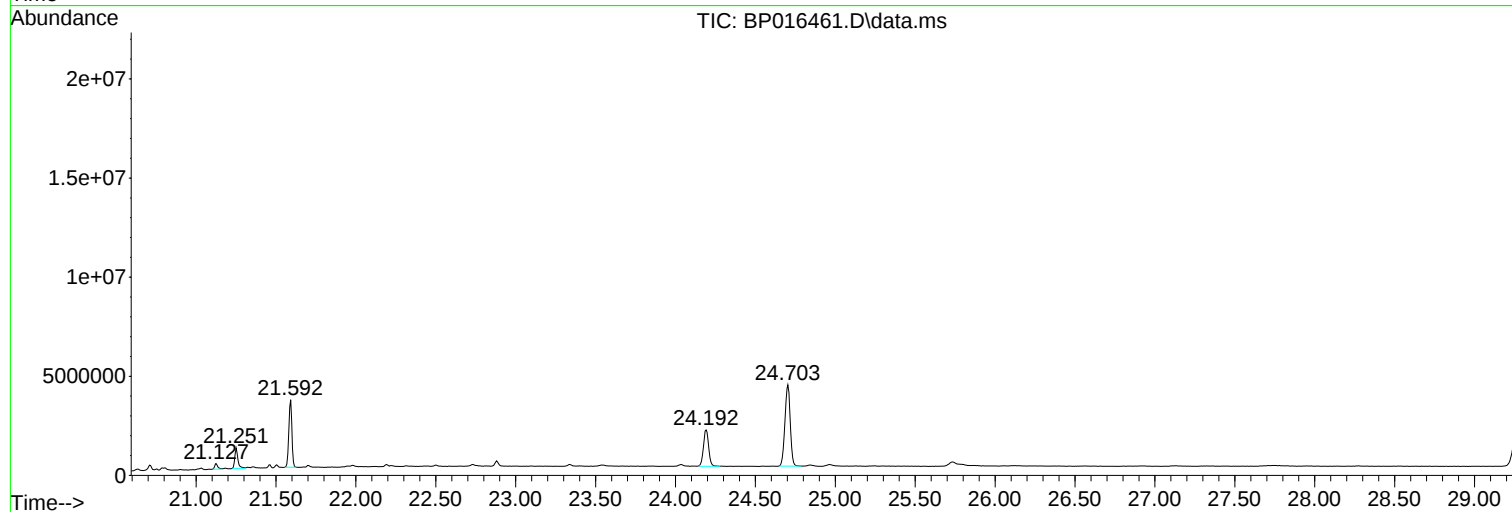
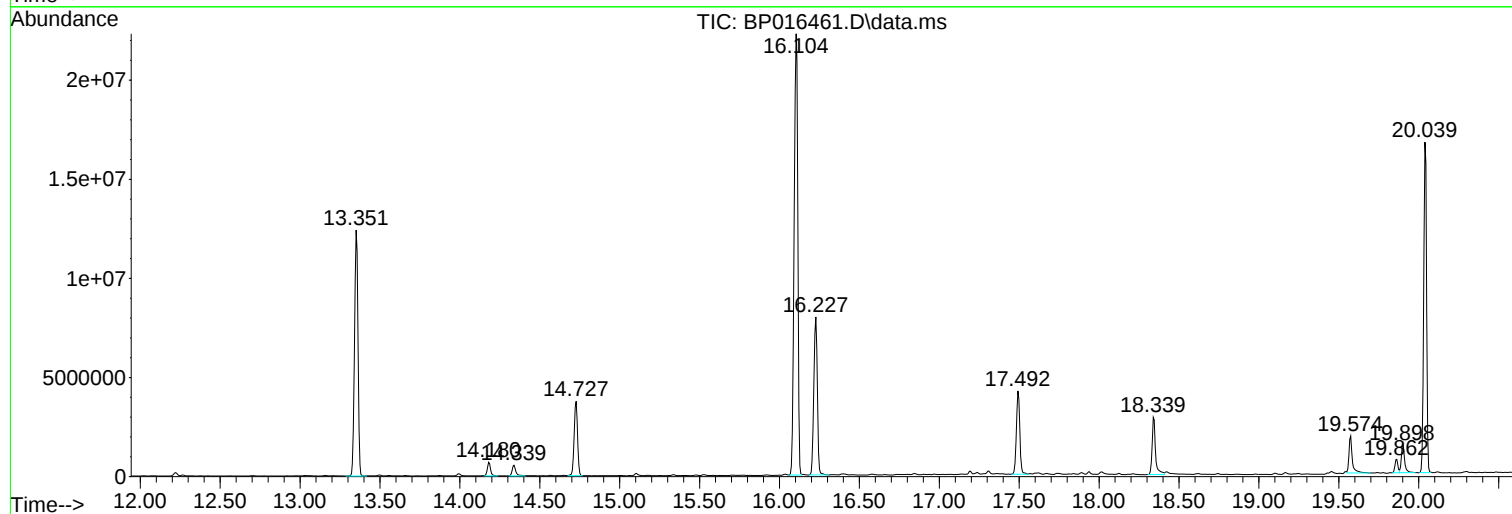
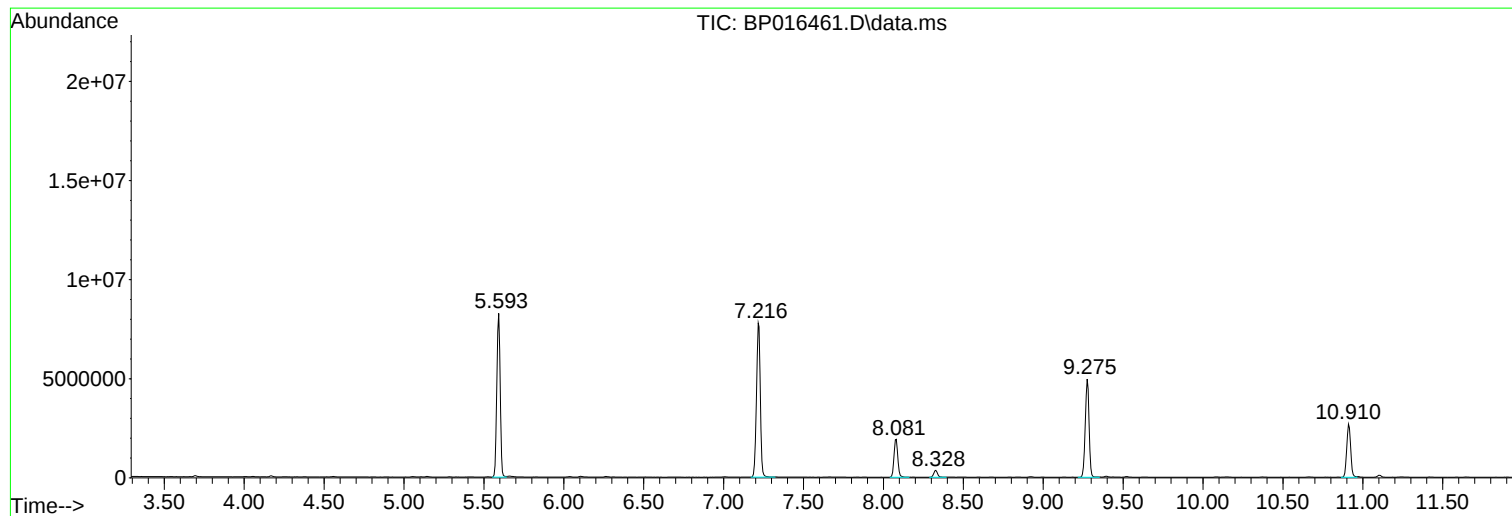
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ClientSampleId :
T842-CT-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.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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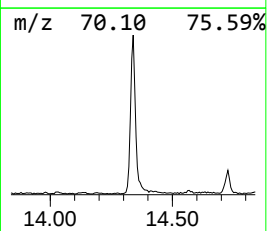
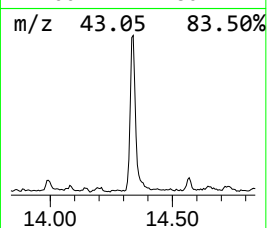
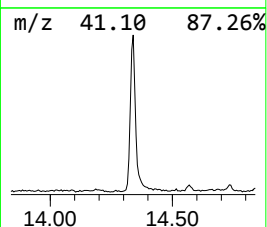
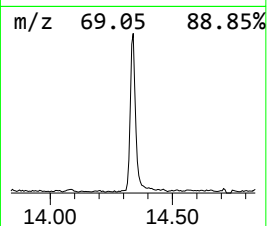
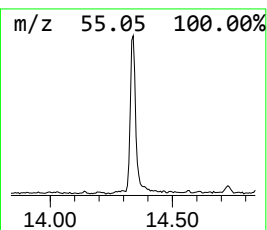
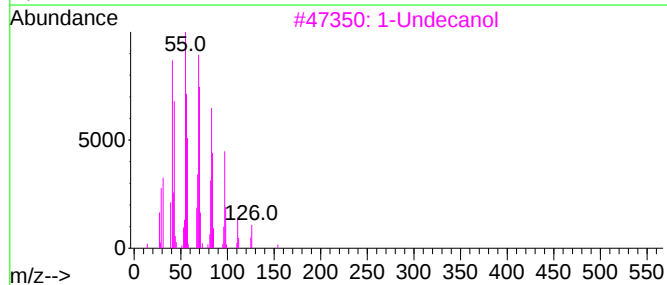
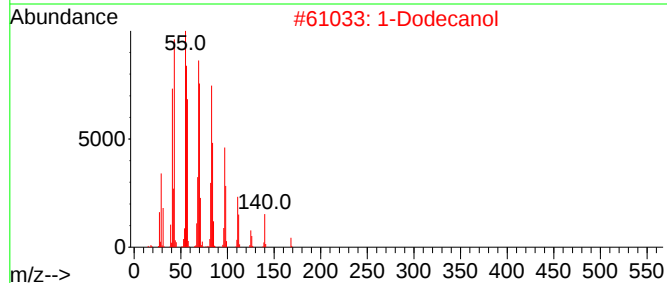
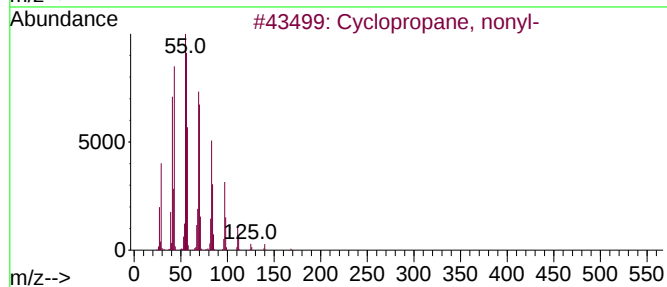
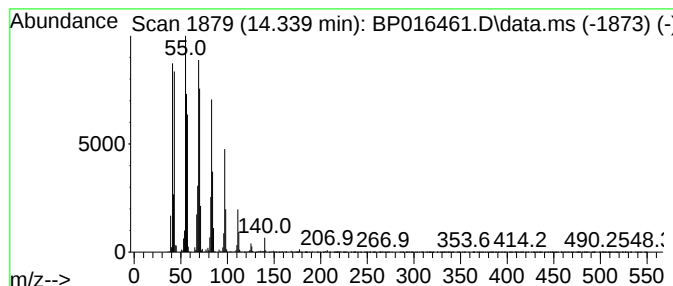
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclopropane, nonyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.339	2.91 ng	804658	Acenaphthene-d10	14.727

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, nonyl-	168	C12H24	074663-85-7	95
2			1-Dodecanol	186	C12H26O	000112-53-8	91
3			1-Undecanol	172	C11H24O	000112-42-5	91
4			Pentadecafluorooctanoic acid, de...	554	C18H21F15O2	1000406-04-0	91
5			Decyl trifluoroacetate	254	C12H21F3O2	000333-88-0	91



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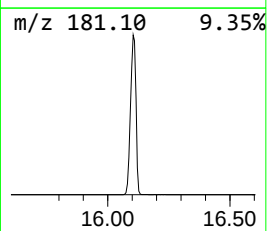
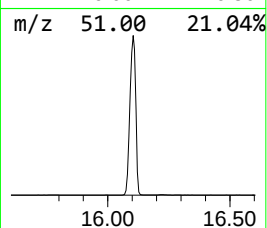
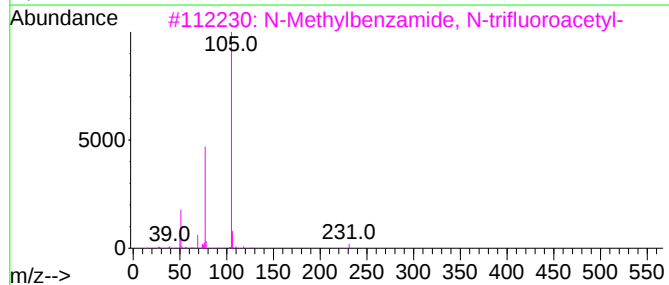
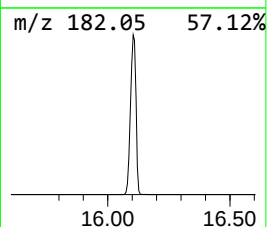
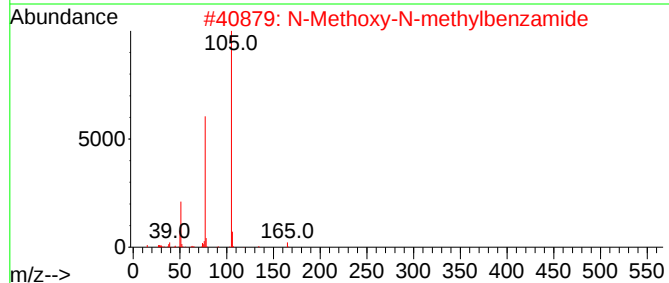
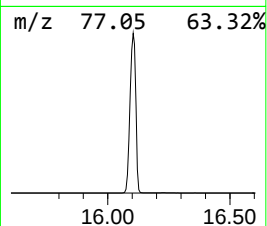
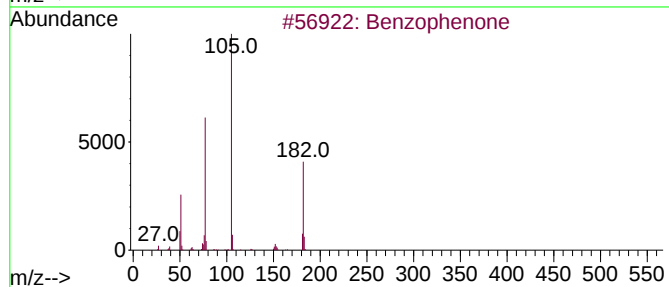
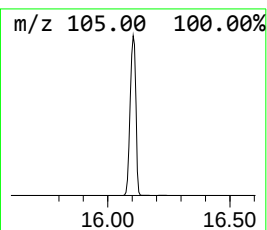
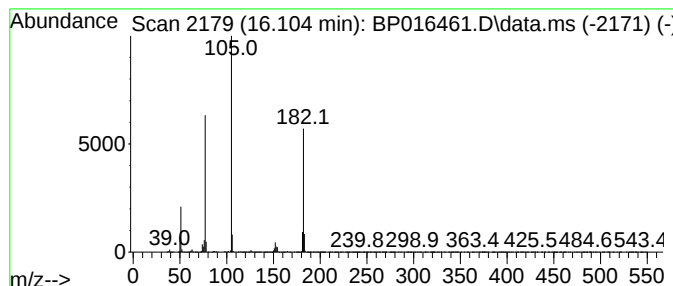
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	129.49 ng	35856900	Acenaphthene-d10	14.727

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
3			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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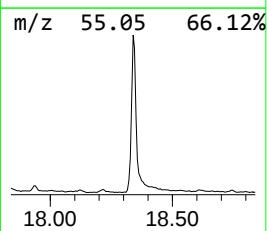
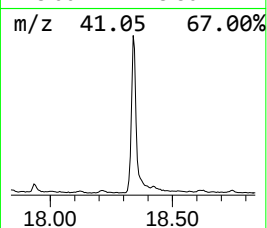
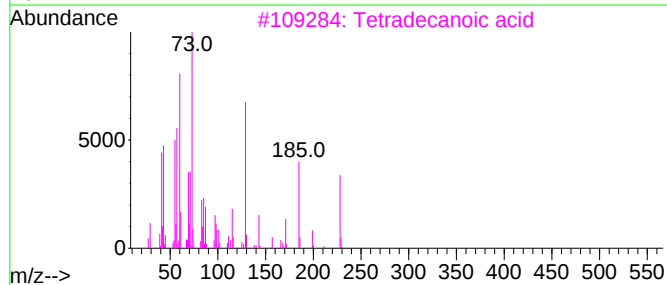
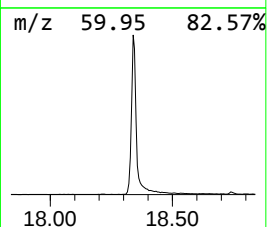
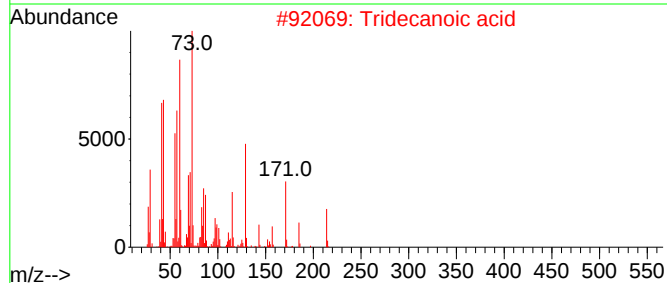
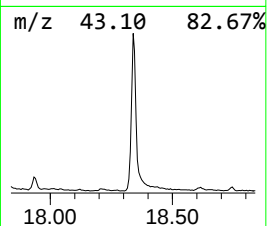
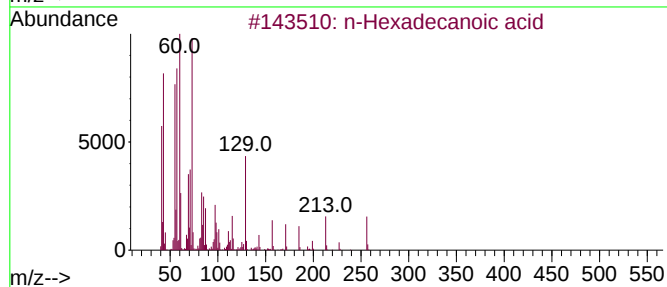
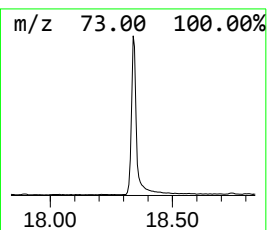
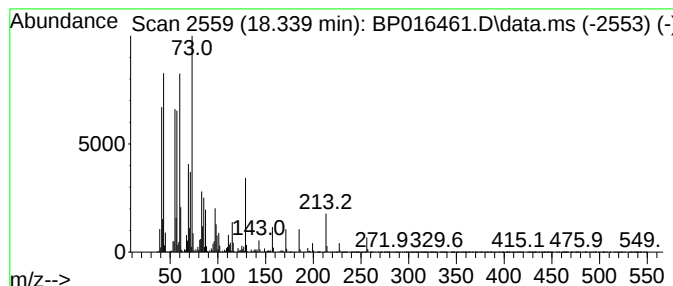
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BNA_P
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.339	13.65 ng	4198930	Phenanthrene-d10		17.492	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	93
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	55



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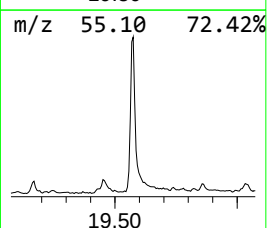
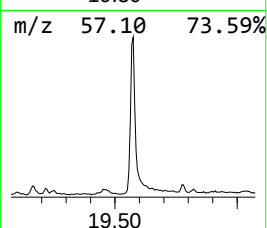
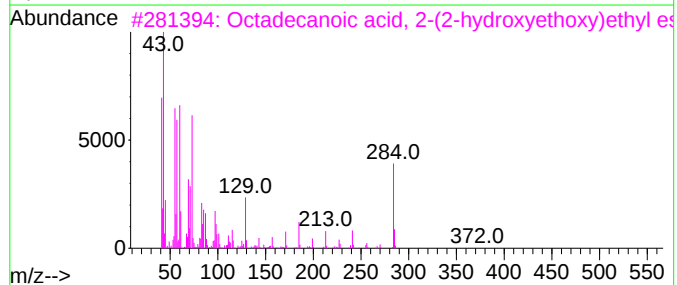
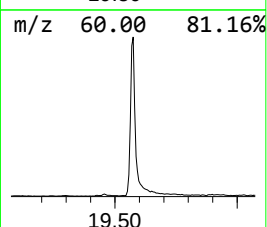
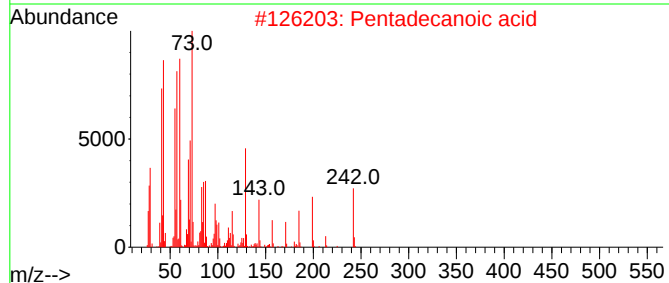
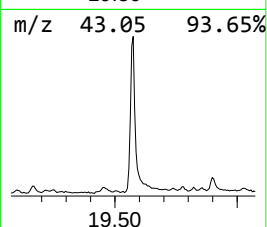
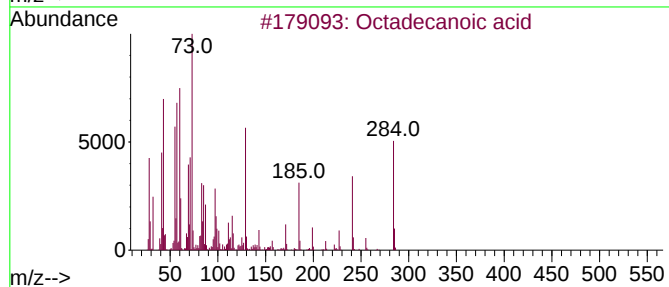
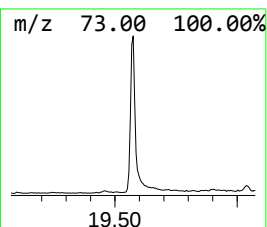
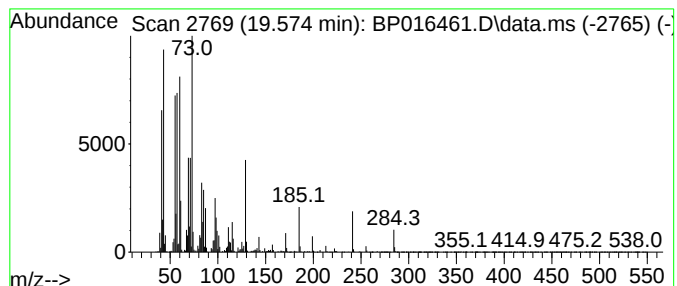
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.574	11.69 ng	2648600	Chrysene-d12	21.592

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	91
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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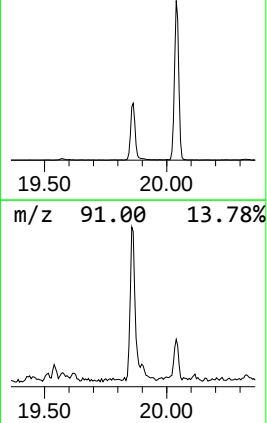
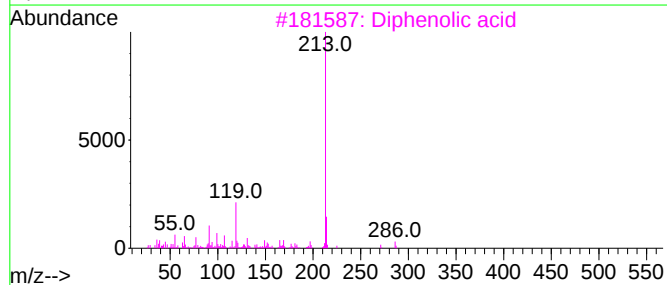
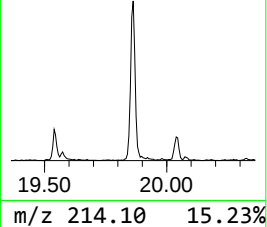
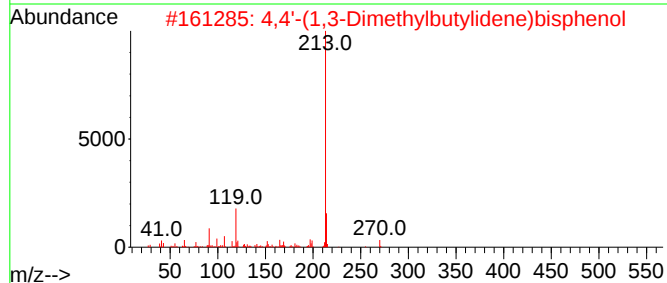
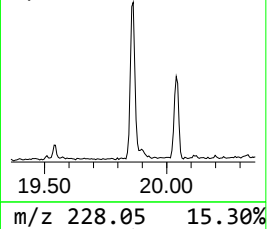
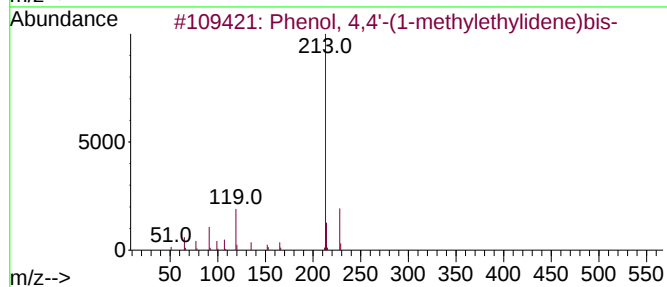
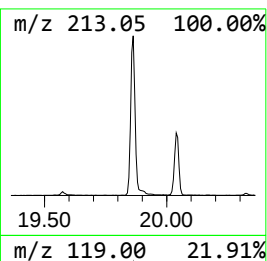
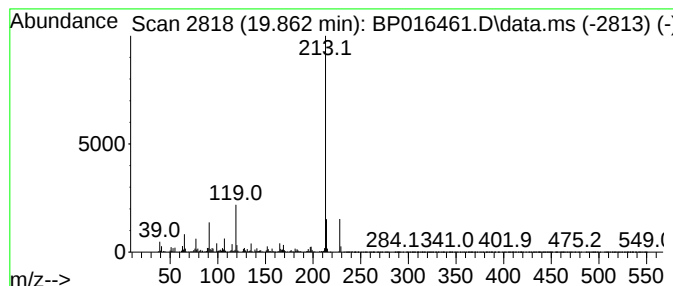
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.862	3.91 ng	884781	Chrysene-d12	21.592

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97
2			4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	80
3			Diphenolic acid	286	C17H18O4	000126-00-1	56
4			2H,8H-Benzo[1,2-b:3,4-b']dipyr...	228	C14H12O3	000523-59-1	52
5			4-Adamantan-1-yl-2-(2-methylprop...	333	C19H27NO2S	1000311-66-6	50



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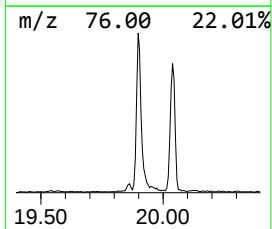
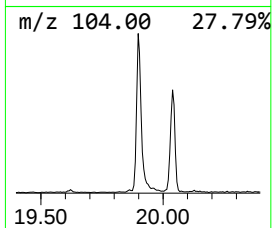
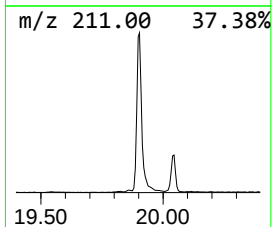
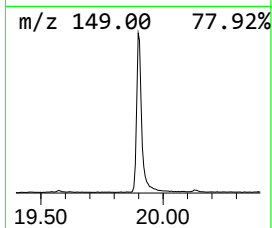
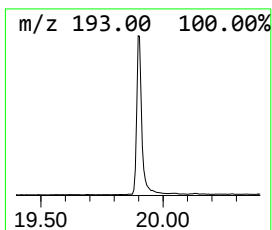
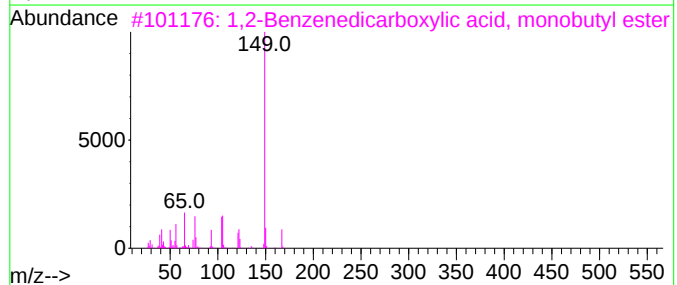
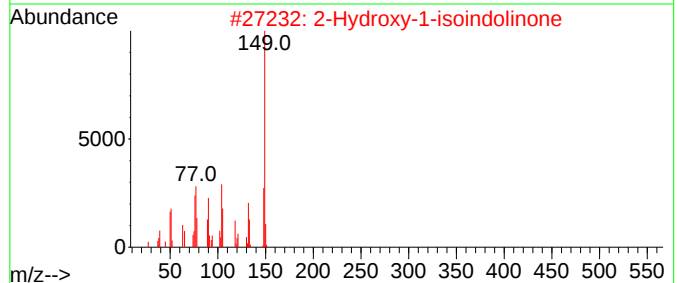
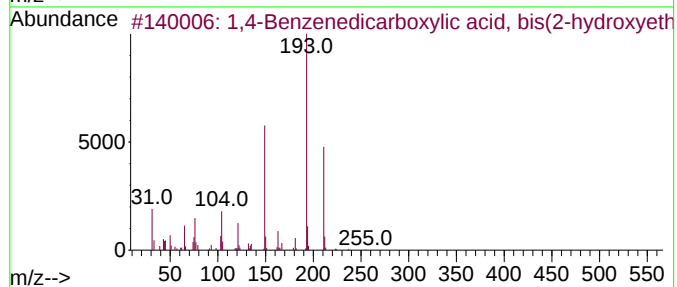
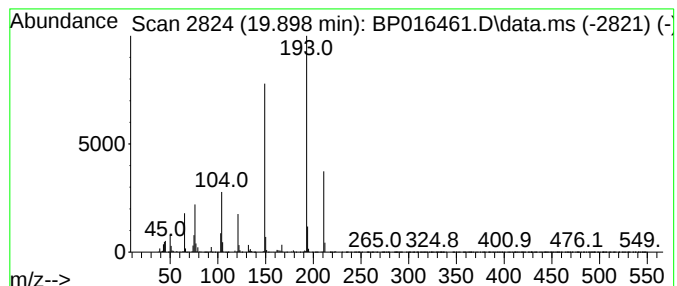
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown19.898 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.898	8.90 ng	2016430	Chrysene-d12	21.592

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	254	C12H14O6	000959-26-2	47
2			2-Hydroxy-1-isoindolinone	149	C8H7NO2	1000289-12-0	38
3			1,2-Benzenedicarboxylic acid, mo...	222	C12H14O4	000131-70-4	27
4			4-(Trifluoroacetyl)benzoic acid	218	C9H5F3O3	058808-59-6	27
5			1,4-Benzenedicarboxylic acid, me...	180	C9H8O4	001679-64-7	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
Data File : BP016461.D
Acq On : 01 Aug 2023 17:54
Operator : MA/JU
Sample : 03715-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
T842-CT-01

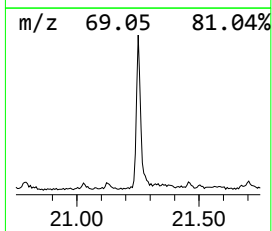
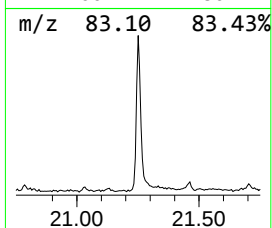
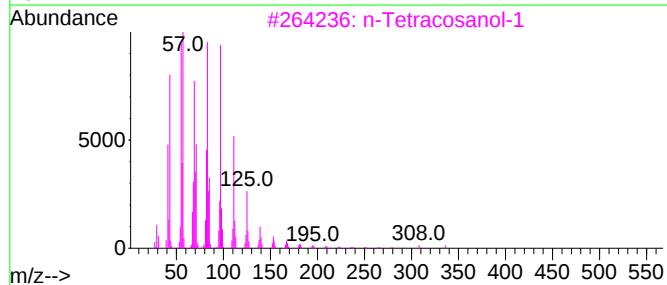
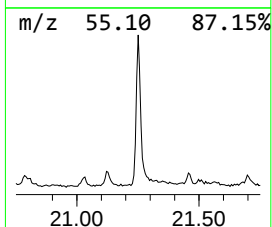
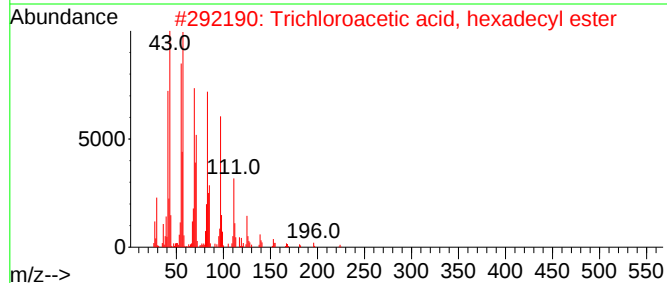
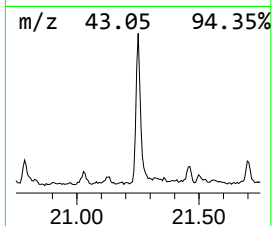
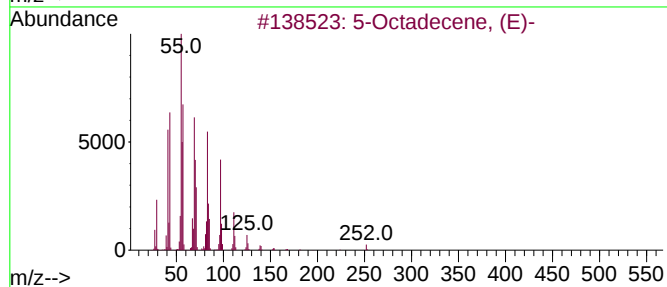
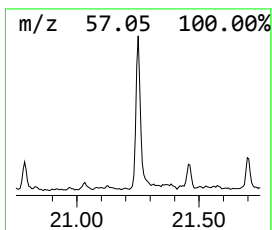
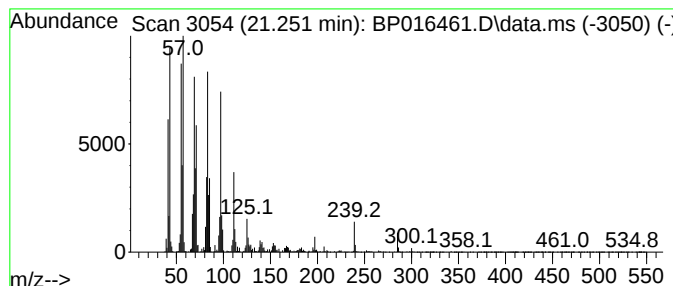
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Octadecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.251	6.07 ng	1375520	Chrysene-d12	21.592

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Octadecene, (E)-	252	C18H36	007206-21-5	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5			Cyclopentadecane	210	C15H30	000295-48-7	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
Data File : BP016461.D
Acq On : 01 Aug 2023 17:54
Operator : MA/JU
Sample : 03715-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
T842-CT-01

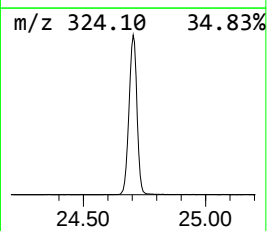
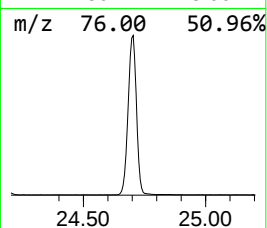
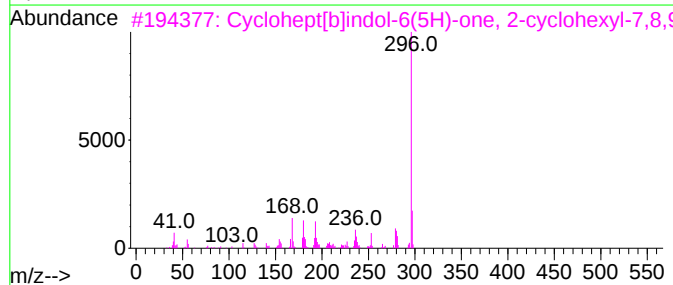
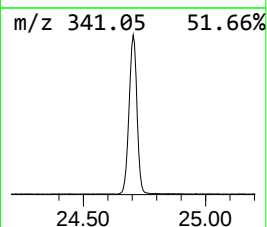
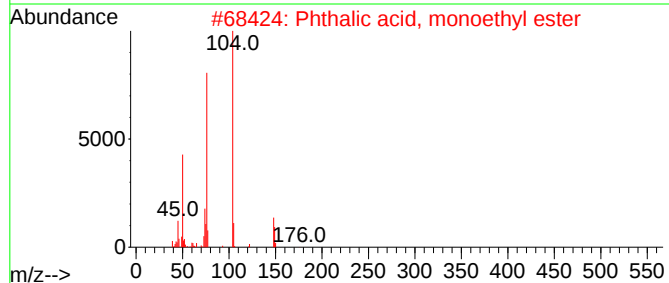
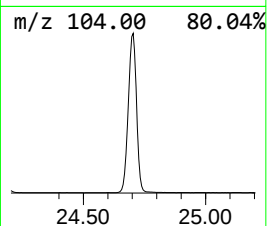
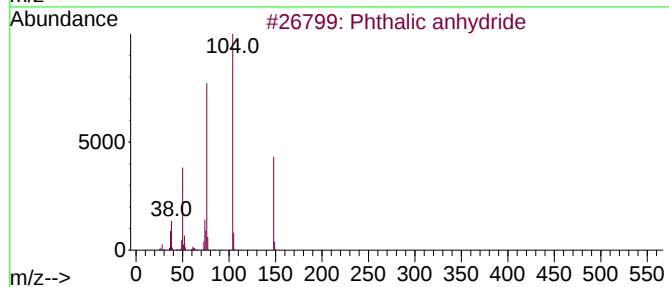
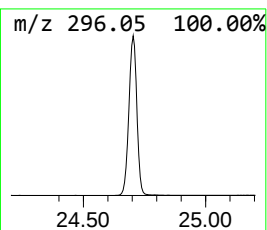
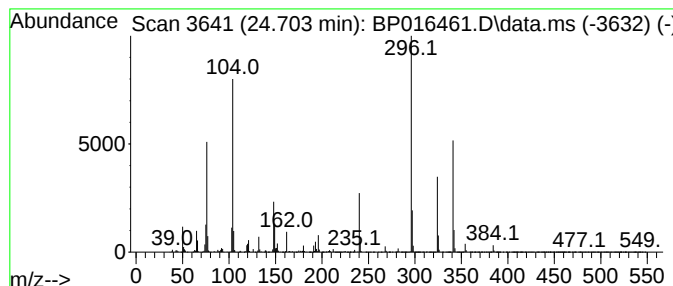
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown24.703 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.703	45.82 ng	9443290	Perylene-d12	24.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic anhydride	148	C8H4O3	000085-44-9	27
2			Phthalic acid, monoethyl ester	194	C10H10O4	002306-33-4	22
3			Cyclohept[b]indol-6(5H)-one, 2-c...	296	C19H24N2O	339284-86-5	14
4			4-[4-(4-Methoxyphenyl)-5-methyl-...	296	C17H16N2O3	394237-61-7	14
5			3-(3',4'-Dimethoxyphenyl)-4-meth...	296	C18H16O4	091787-20-1	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
Data File : BP016461.D
Acq On : 01 Aug 2023 17:54
Operator : MA/JU
Sample : 03715-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
T842-CT-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.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
Cyclopropane, n...	14.339	2.9	ng	804658	3	14.727	5538110	20.0
Benzophenone	16.104	129.5	ng	35856900	3	14.727	5538110	20.0
n-Hexadecanoic ...	18.339	13.7	ng	4198930	4	17.492	6154130	20.0
Octadecanoic acid	19.574	11.7	ng	2648600	5	21.592	4530420	20.0
Phenol, 4,4'-(1...	19.862	3.9	ng	884781	5	21.592	4530420	20.0
unknown19.898	19.898	8.9	ng	2016430	5	21.592	4530420	20.0
5-Octadecene, (E)-	21.251	6.1	ng	1375520	5	21.592	4530420	20.0
unknown24.703	24.703	45.8	ng	9443290	6	24.192	4121950	20.0