

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
 Data File : BF128557.D
 Acq On : 28 May 2022 19:38
 Operator : CG\JU
 Sample : N2931-02
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P009-SS003-0612-01

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_F\Methods\8270-BF052622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128557.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.928	104	109	115	rBV	38634	60464	1.68%	0.218%
2	5.051	466	470	480	rVB	129572	156540	4.35%	0.564%
3	5.451	532	538	541	rBV	3078077	3048657	84.71%	10.975%
4	6.293	676	681	688	rBV2	42783	73037	2.03%	0.263%
5	6.463	704	710	712	rBV	2823809	3161298	87.84%	11.380%
6	6.575	726	729	741	rBV	48881	55834	1.55%	0.201%
7	6.840	770	774	777	rBV	1063061	923184	25.65%	3.323%
8	7.398	864	869	872	rBV	2371218	2089483	58.06%	7.522%
9	8.116	987	991	995	rBV	1297366	1189458	33.05%	4.282%
10	9.198	1169	1175	1178	rBV	4217323	3599116	100.00%	12.956%
11	9.828	1277	1282	1285	rBV	2072871	1666048	46.29%	5.998%
12	9.875	1286	1290	1294	rVV	1658858	1328308	36.91%	4.782%
13	10.663	1420	1424	1427	rBV	2519017	2134807	59.31%	7.685%
14	10.745	1433	1438	1440	rBV	104556	147322	4.09%	0.530%
15	10.775	1440	1443	1446	rVB	1083701	1082402	30.07%	3.897%
16	11.363	1539	1543	1546	rBV	1504911	1246769	34.64%	4.488%
17	11.757	1604	1610	1614	rBV	52290	47589	1.32%	0.171%
18	11.886	1629	1632	1637	rBV	178420	186125	5.17%	0.670%
19	12.675	1763	1766	1774	rBV	42463	47397	1.32%	0.171%
20	12.951	1809	1813	1816	rBV	3314636	2888061	80.24%	10.397%
21	13.904	1971	1975	1985	rBV4	64833	169833	4.72%	0.611%
22	13.998	1987	1991	1995	rVV	902746	900566	25.02%	3.242%
23	14.033	1995	1997	2000	rVB3	47372	44722	1.24%	0.161%
24	14.098	2004	2008	2016	rVV	466980	487972	13.56%	1.757%
25	14.868	2135	2139	2144	rVB	86049	89008	2.47%	0.320%
26	15.463	2235	2240	2246	rBV	672282	867096	24.09%	3.121%
27	15.974	2320	2327	2331	rVB3	45226	87543	2.43%	0.315%

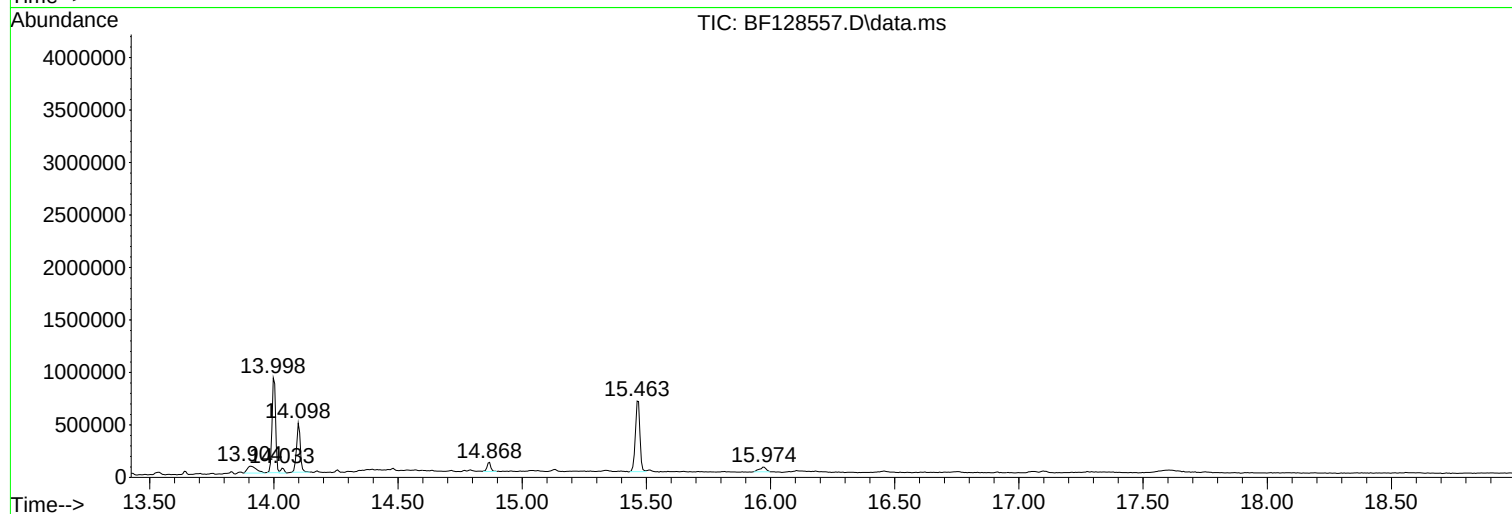
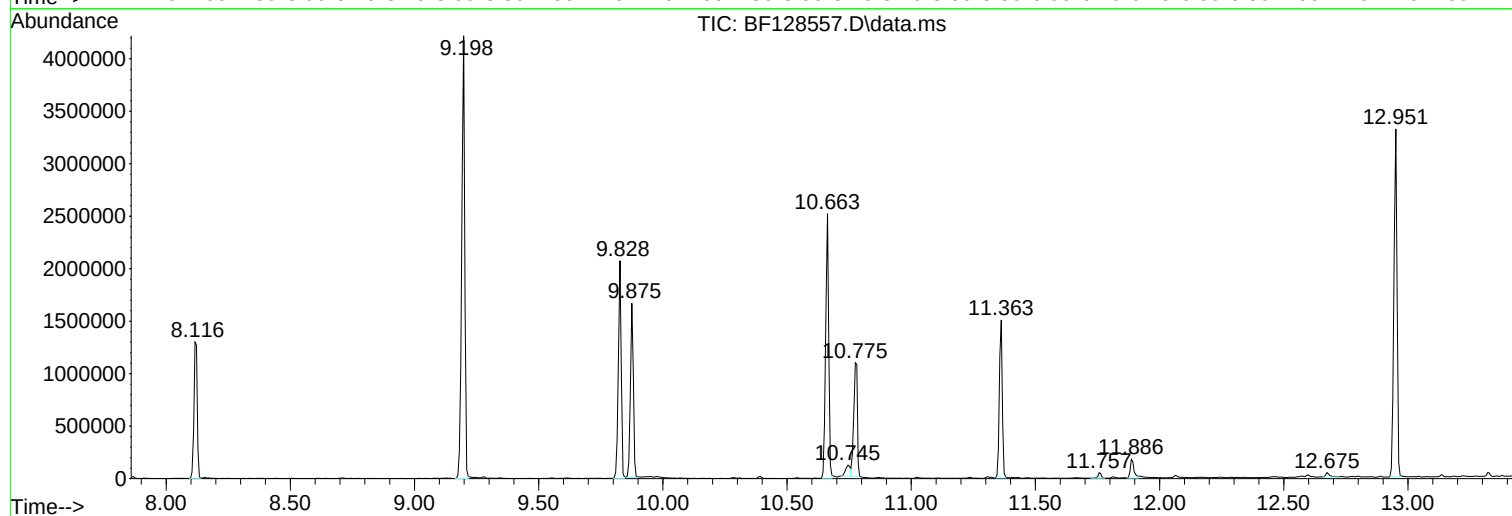
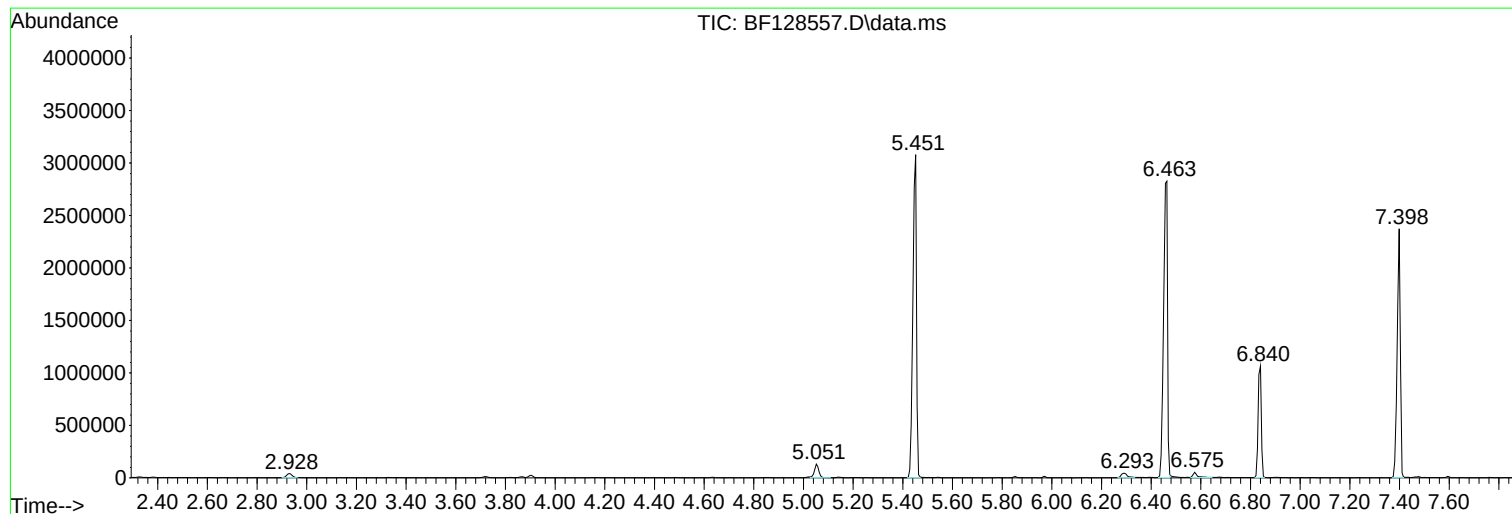
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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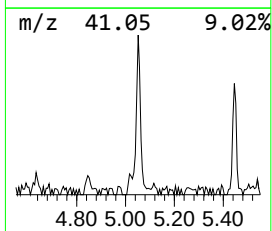
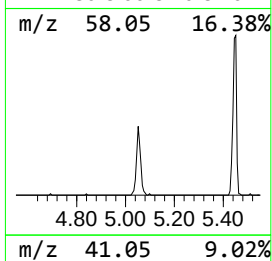
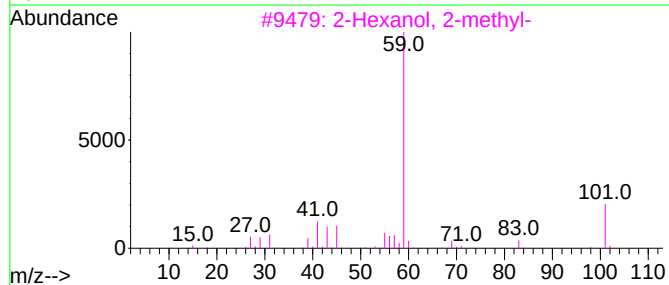
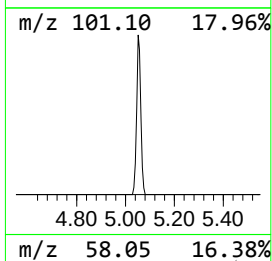
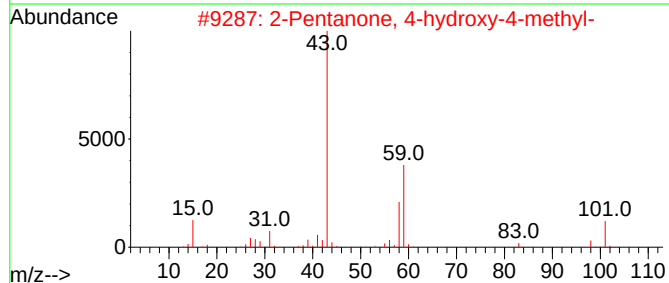
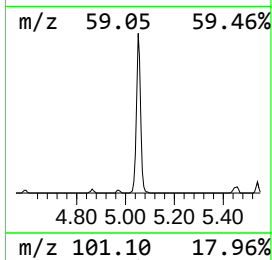
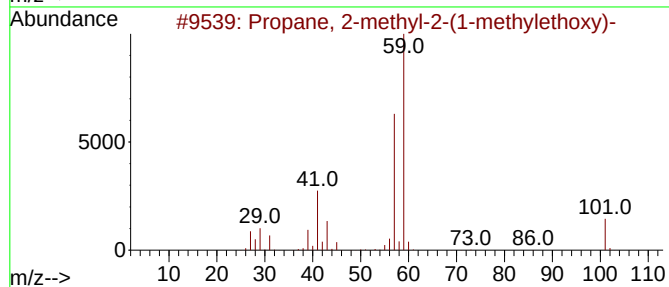
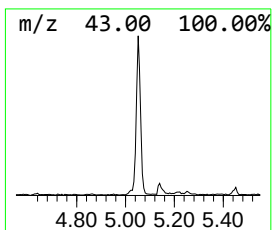
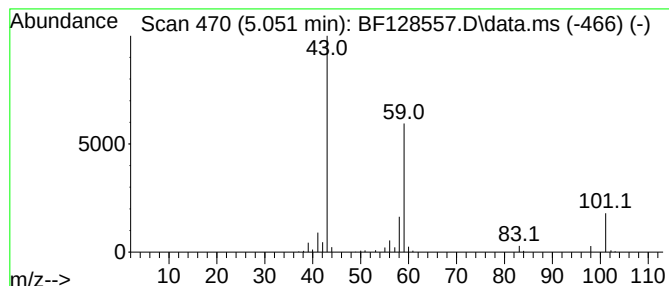
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2-methyl-2-(1-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	3.39 ng	156540	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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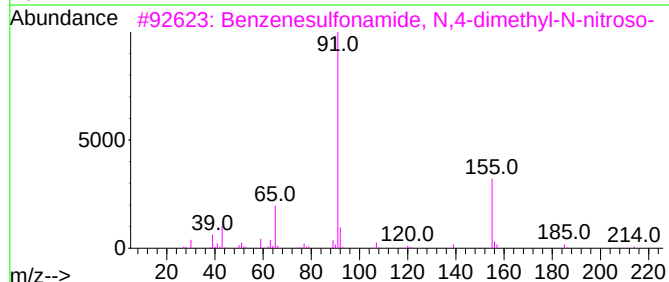
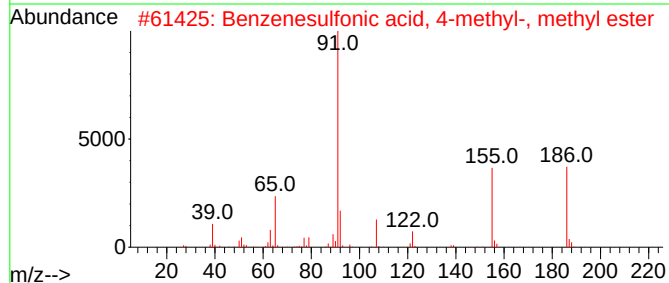
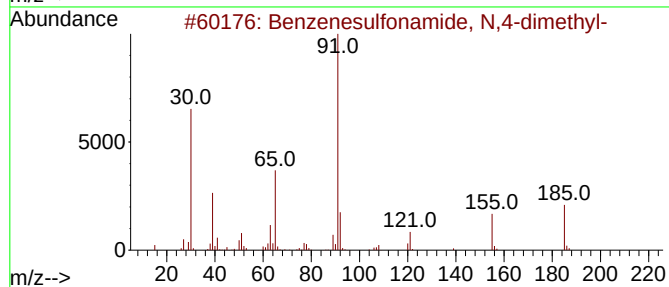
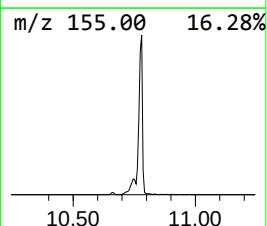
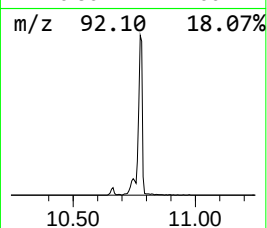
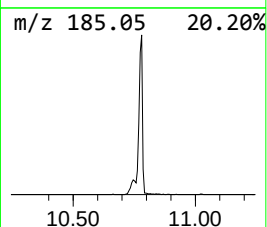
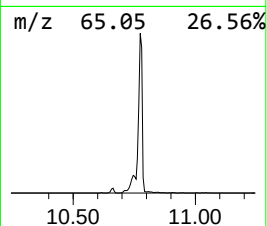
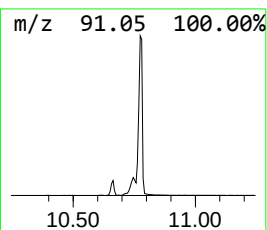
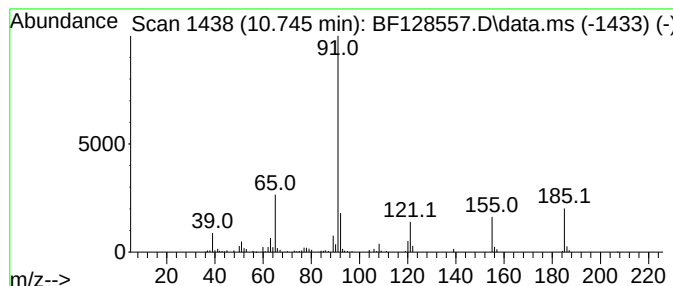
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzenesulfonamide, N,4-dim... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.745	2.36 ng	147322	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	90
2			Benzenesulfonic acid, 4-methyl-,...	186	C8H10O3S	000080-48-8	50
3			Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	47
4			(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	43
5			Benzeneethanamine	121	C8H11N	000064-04-0	38



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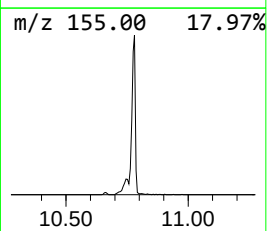
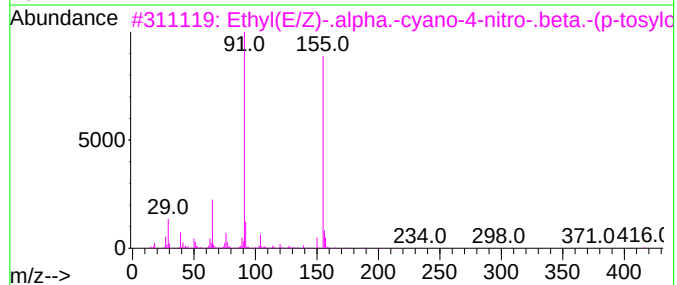
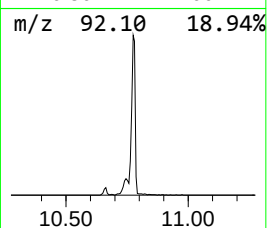
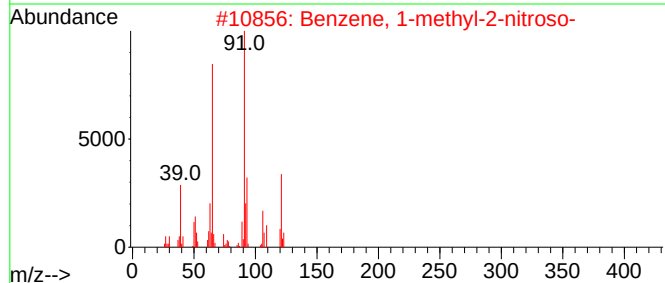
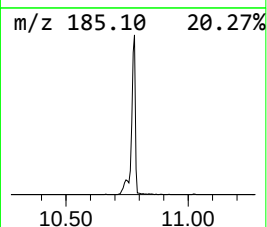
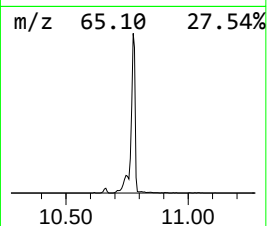
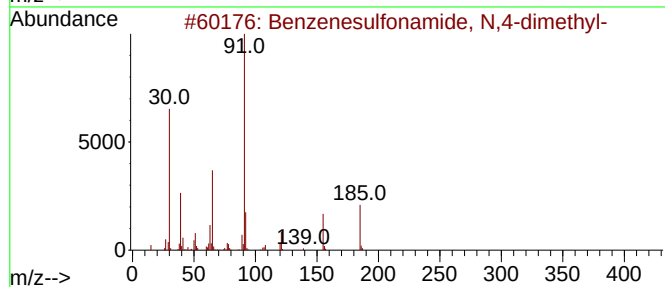
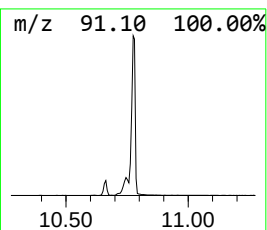
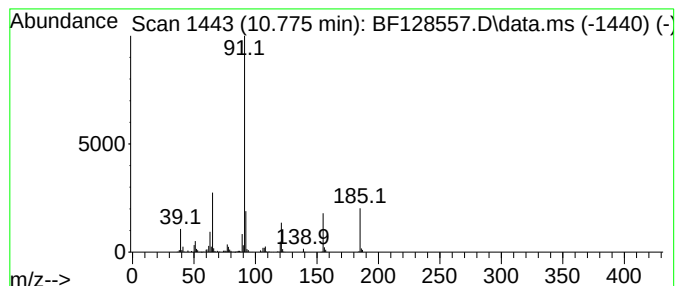
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzene, 1-methyl-2-nitroso- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.775	17.36 ng	1082400	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	96
2			Benzene, 1-methyl-2-nitroso-	121	C7H7NO	000611-23-4	52
3			Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	50
4			Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	50
5			4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	47



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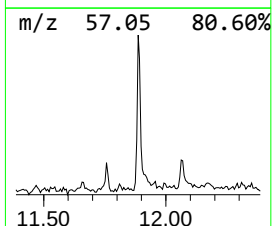
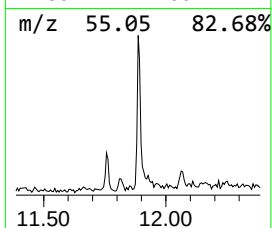
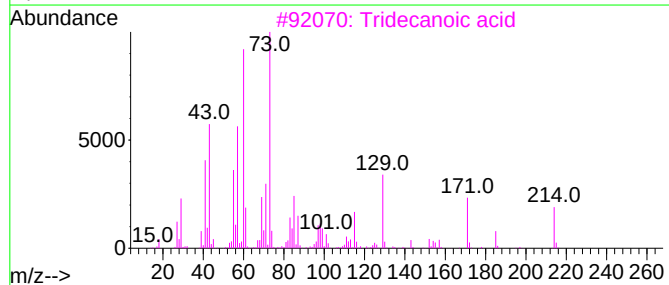
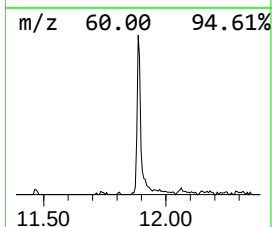
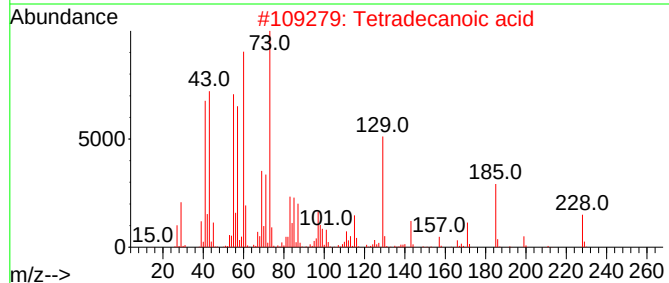
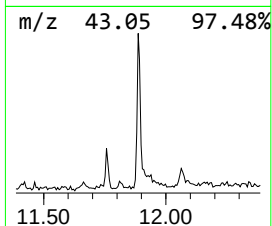
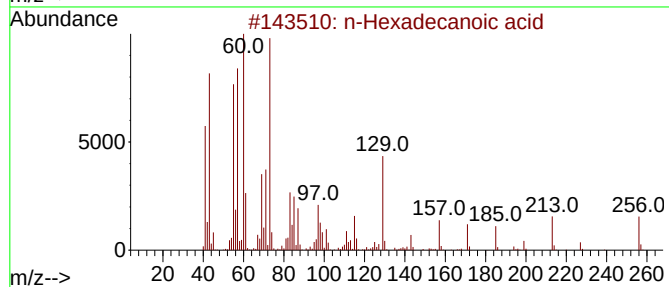
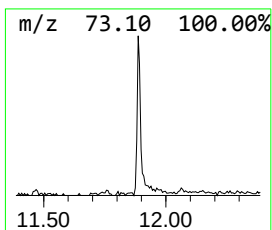
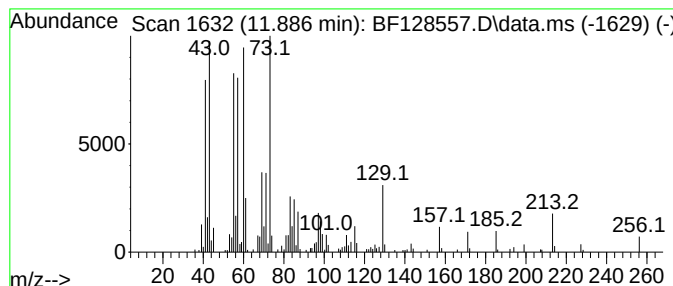
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	2.99 ng	186125	Phenanthrene-d10	11.363

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	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5		Undecanoic acid	186	C11H22O2	000112-37-8	59



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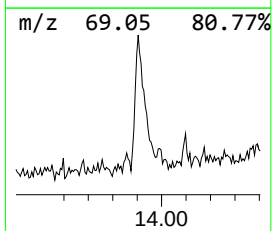
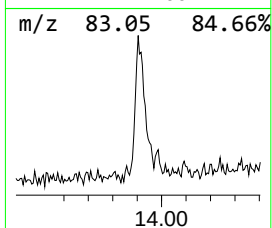
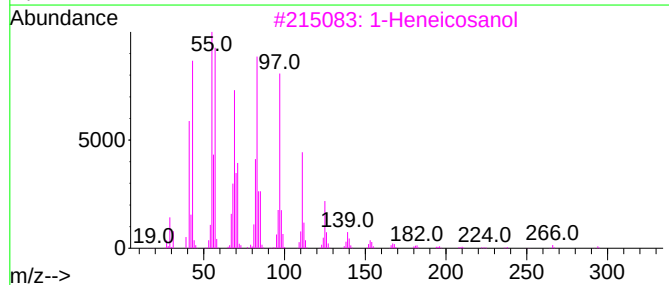
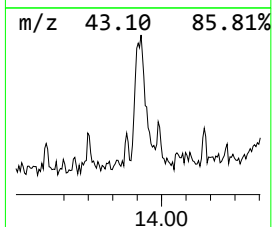
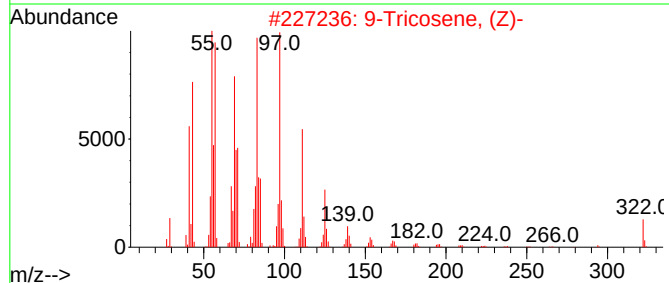
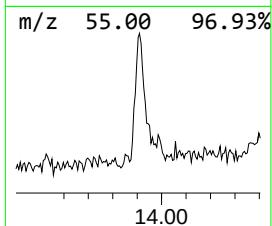
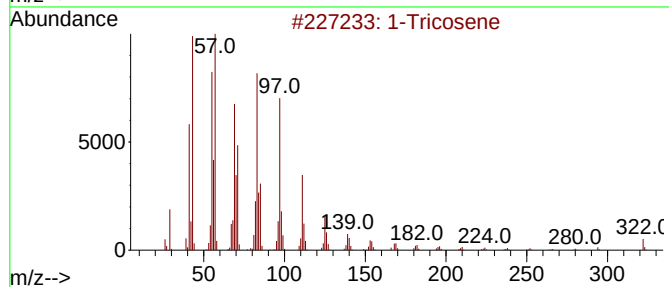
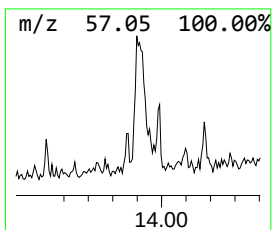
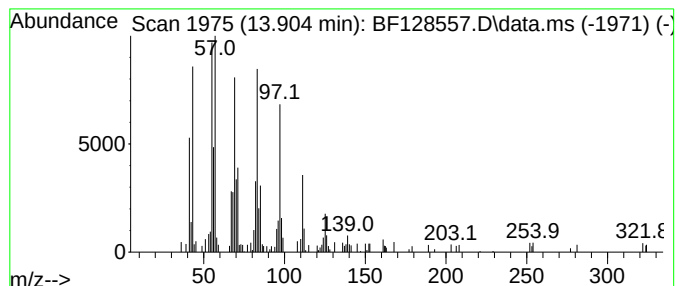
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Tricosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.77 ng	169833	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene			322	C23H46	018835-32-0	98
2	9-Tricosene, (Z)-			322	C23H46	027519-02-4	96
3	1-Heneicosanol			312	C21H44O	015594-90-8	95
4	11-Tricosene			322	C23H46	052078-56-5	94
5	1-Hexacosene			364	C26H52	018835-33-1	93



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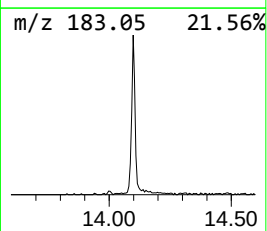
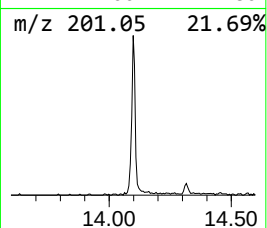
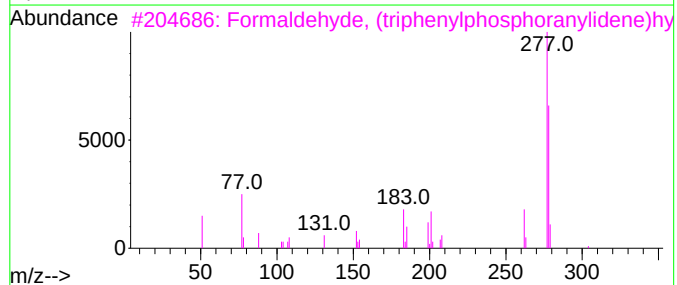
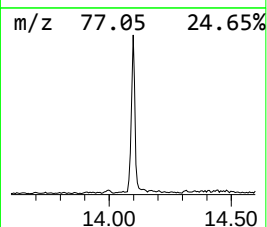
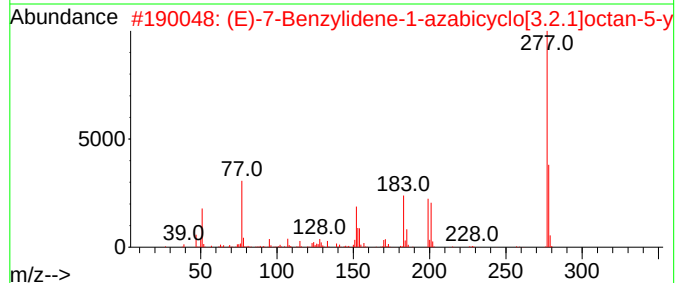
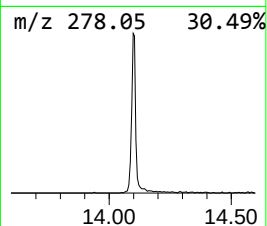
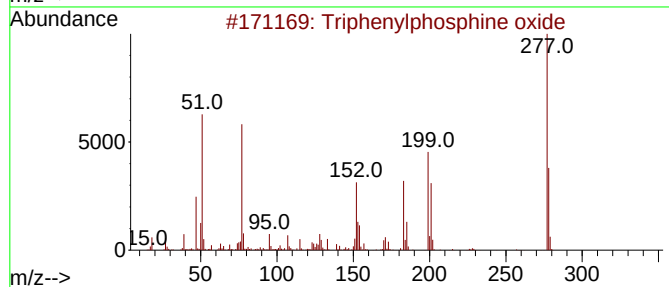
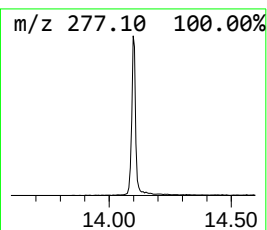
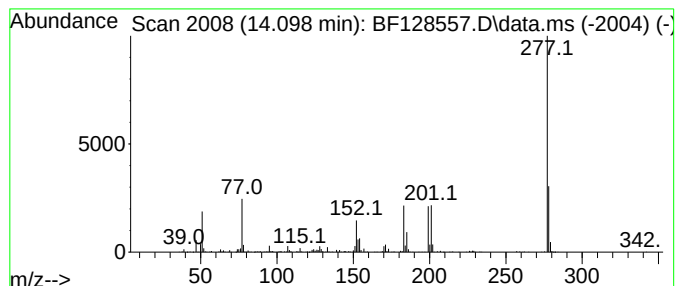
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	10.84 ng	487972	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	76
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128557.D
Acq On : 28 May 2022 19:38
Operator : CG\JU
Sample : N2931-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P009-SS003-0612-01

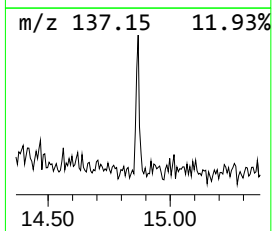
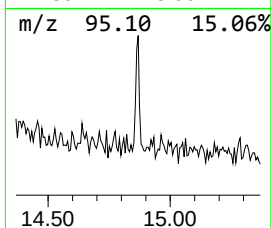
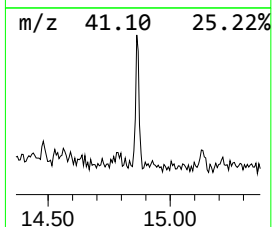
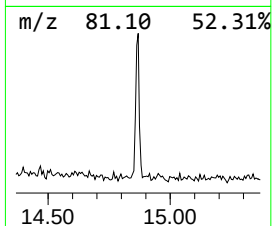
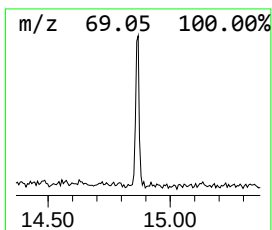
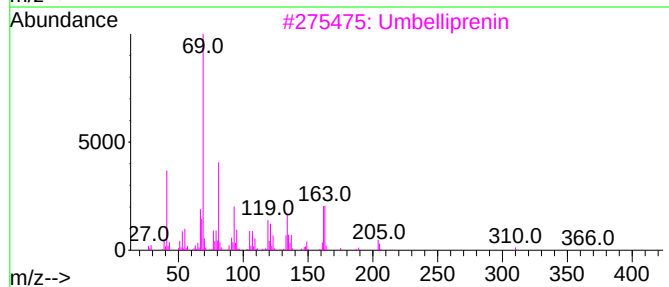
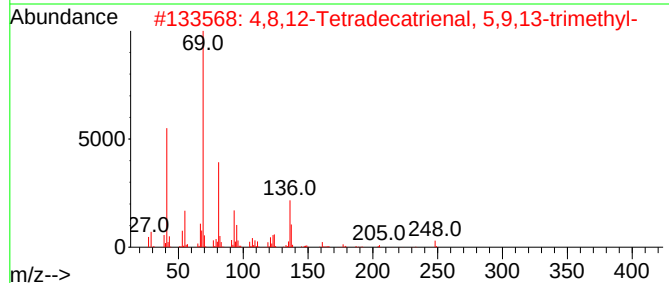
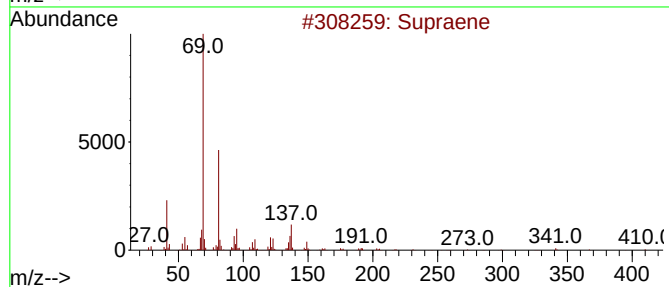
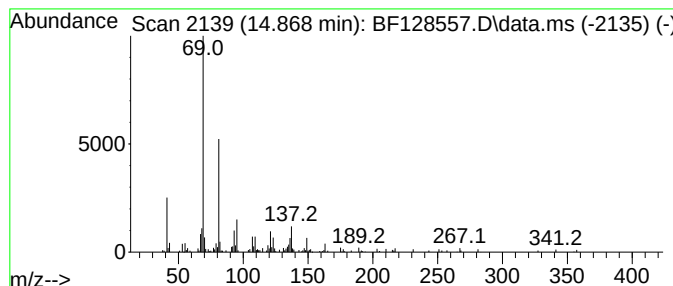
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	2.05 ng	89008	Perylene-d12	15.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
3			Umbelliprenin	366	C24H30O3	023838-17-7	72
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128557.D
Acq On : 28 May 2022 19:38
Operator : CG\JU
Sample : N2931-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P009-SS003-0612-01

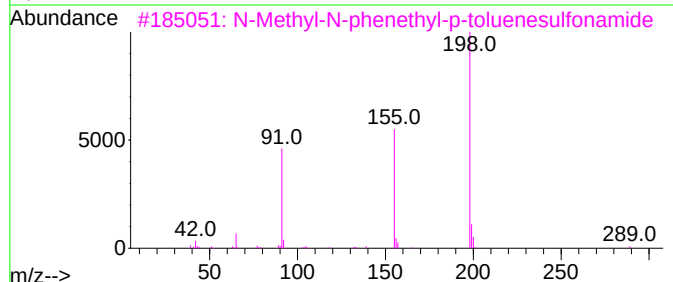
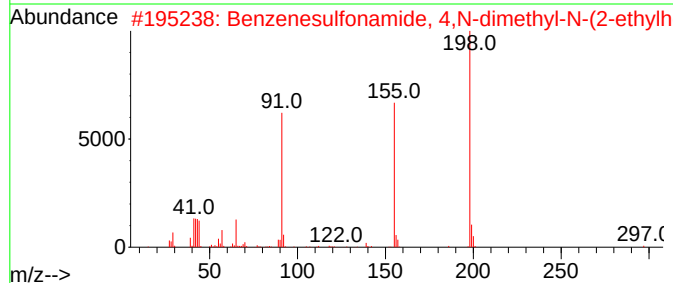
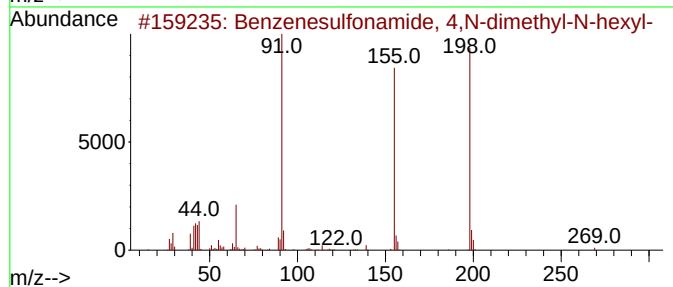
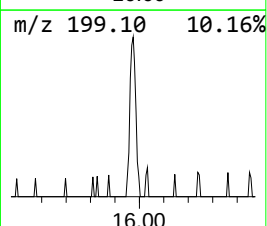
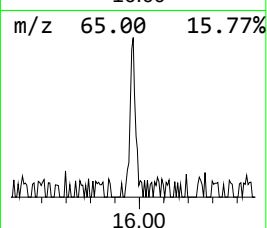
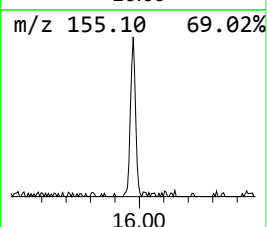
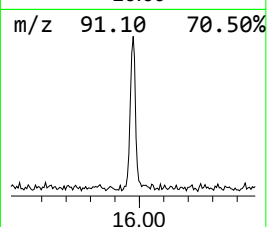
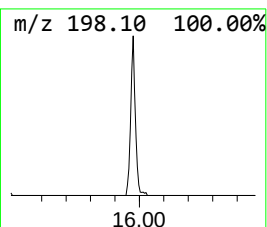
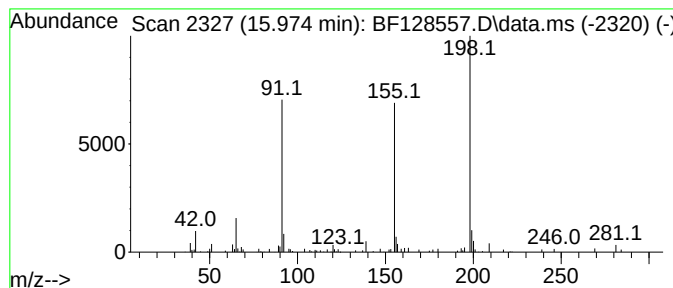
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzenesulfonamide, 4,N-dim... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	2.02 ng	87543	Perylene-d12	15.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, 4,N-dimethyl...	269	C14H23NO2S	1000421-17-3	93
2			Benzenesulfonamide, 4,N-dimethyl...	297	C16H27NO2S	1000421-18-3	86
3			N-Methyl-N-phenethyl-p-toluenesu...	289	C16H19NO2S	025566-59-0	86
4			Benzenesulfonamide, 4,N-dimethyl...	283	C15H25NO2S	1000421-17-4	86
5			Benzenesulfonamide, 4,N-dimethyl...	297	C16H27NO2S	1000421-17-5	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128557.D
Acq On : 28 May 2022 19:38
Operator : CG\JU
Sample : N2931-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P009-SS003-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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
Propane, 2-meth...	5.051	3.4	ng	156540	1	6.840	923184	20.0
Benzenesulfonam...	10.745	2.4	ng	147322	4	11.363	1246770	20.0
Benzene, 1-meth...	10.775	17.4	ng	1082400	4	11.363	1246770	20.0
n-Hexadecanoic ...	11.886	3.0	ng	186125	4	11.363	1246770	20.0
1-Tricosene	13.904	3.8	ng	169833	5	13.998	900566	20.0
Triphenylphosph...	14.098	10.8	ng	487972	5	13.998	900566	20.0
Supraene	14.868	2.0	ng	89008	6	15.469	867096	20.0
Benzenesulfonam...	15.974	2.0	ng	87543	6	15.469	867096	20.0