LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138378.D
Acq On : 27 Jun 2024 21:09
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-W-1

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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138378.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	8	14	21	rBV	1838171	2302832	74.94%	7.747%
2	2.281	29	33	39	rVB	26607	35885	1.17%	0.121%
3	3.398	219	223	234	rBV	72959	185031	6.02%	0.622%
4	5.098	508	512	520	rVB	238356	253296	8.24%	0.852%
5	5.510	577	582	585	rBV	3119530	3072799	100.00%	10.337%
6	6.516	748	753	756	rBV	3357160	2978864	96.94%	10.021%
7	6.704	782	785	790	rBV	71568	63982	2.08%	0.215%
8	6.881	811	815	818	rBV	1645995	1280910	41.69%	4.309%
9	6.939	821	825	832	rBV	39200	36794	1.20%	0.124%
10	7.439	902	910	913	rBV	2234757	1938513	63.09%	6.521%
11	7.692	949	953	960	rVB	133141	103249	3.36%	0.347%
12	8.163	1029	1033	1036	rBV	1798350	1579910	51.42%	5.315%
13	8.375	1063	1069	1075	rVB	38553	40471	1.32%	0.136%
14	8.469	1081	1085	1094	rVB	214235	184547	6.01%	0.621%
15	9.233	1211	1215	1218	rBV	3756407	3019531	98.27%	10.158%
16	9.910	1327	1330	1334	rBV	1713919	1443940	46.99%	4.857%
17	9.945	1334	1336	1340	rVB	49992	41095	1.34%	0.138%
18	10.010	1342	1347	1353	rVB	82285	108179	3.52%	0.364%
19	10.457	1420	1423	1428	rBV	45005	36448	1.19%	0.123%
20	10.698	1460	1464	1475	rBV	1964586	1595003	51.91%	5.366%
21	10.804	1479	1482	1490	rVB	189276	192299	6.26%	0.647%
22	11.398	1579	1583	1585	rBV	1497999	1224516	39.85%	4.119%
23	11.421	1585	1587	1590	rVV	344691	254429	8.28%	0.856%
24	11.469	1590	1595	1599	rVB	84877	87729	2.86%	0.295%
25	11.627	1616	1622	1629	rBV	27291	39255	1.28%	0.132%
26	11.921	1669	1672	1678	rVB2	206776	190827	6.21%	0.642%
27	12.010	1684	1687	1689	rBV	73313	72416	2.36%	0.244%
28	12.445	1758	1761	1764	rBV	39629	41410	1.35%	0.139%
29	12.480	1764	1767	1773	rVB4	29499	46653	1.52%	0.157%
30	12.610	1785	1789	1792	rBV	600782	489354	15.93%	1.646%
31	12.704	1802	1805	1809	rBV	78174	82097	2.67%	0.276%
32	12.839	1822	1828	1833	rVB	481857	512015	16.66%	1.722%
33	12.980	1848	1852	1855	rBV	3216966	2582828	84.05%	8.689%
34	13.057	1861	1865	1868	rBV3	28638	47130	1.53%	0.159%
35	13.163	1881	1883	1886	rVB	80559	66584	2.17%	0.224%
36	13.233	1892	1895	1897	rVB	61771	50159	1.63%	0.169%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138378.D
Acq On : 27 Jun 2024 21:09
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.268	1898	1901	1904	rVV2	48483	44776	1.46%	0.151%
38	13.392	1919	1922	1925	rBV	34624	40002	1.30%	0.135%
39	13.833	1995	1997	2001	rBV2	28736	37806	1.23%	0.127%
40	13.874	2001	2004	2015	rVB2	213210	253060	8.24%	0.851%
41	14.033	2026	2031	2034	rBV2	1489647	1500494	48.83%	5.048%
42	14.057	2034	2035	2041	rVB	232149	180405	5.87%	0.607%
43	14.504	2108	2111	2115	rBV2	56348	82288	2.68%	0.277%
44	15.074	2204	2208	2218	rVB	161131	305306	9.94%	1.027%
45	15.439	2267	2270	2276	rVB	126001	142319	4.63%	0.479%
46	15.504	2277	2281	2285	rBV	726591	859462	27.97%	2.891%

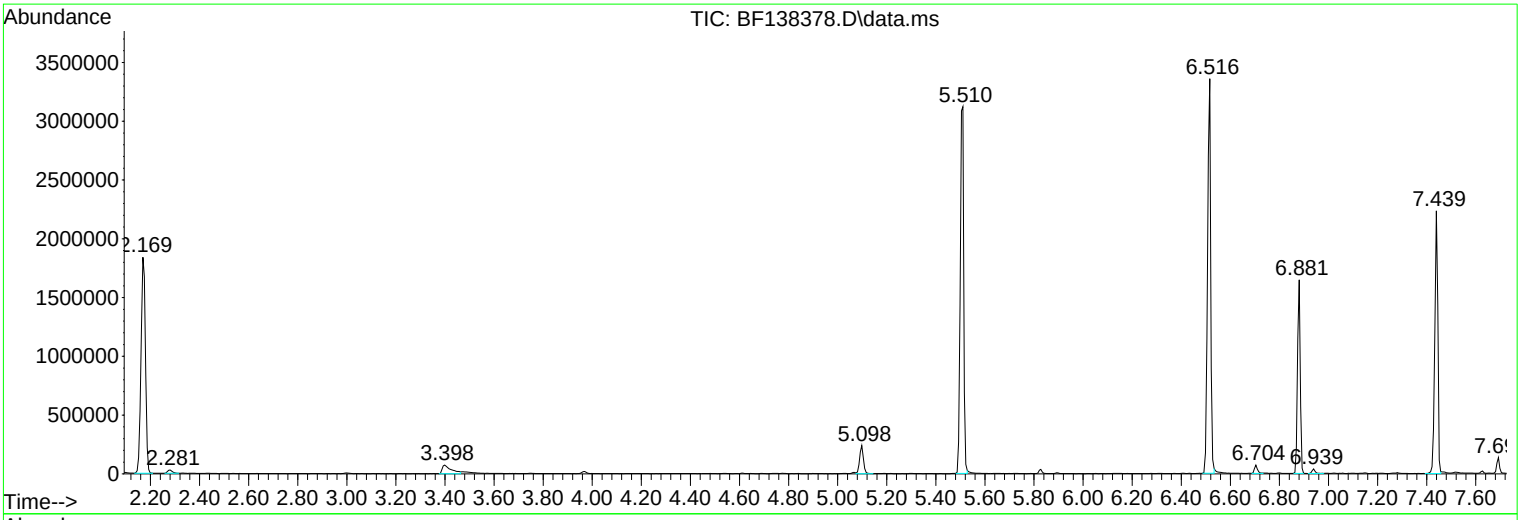
Sum of corrected areas: 29726898

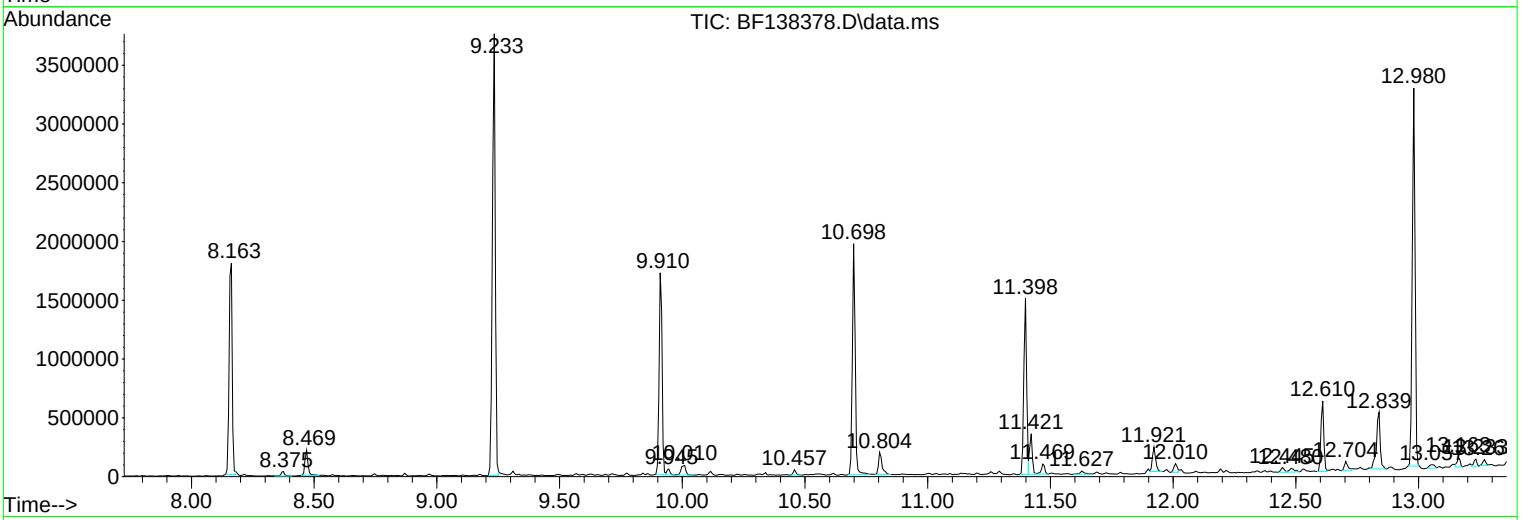
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138378.D
Acq On : 27 Jun 2024 21:09
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

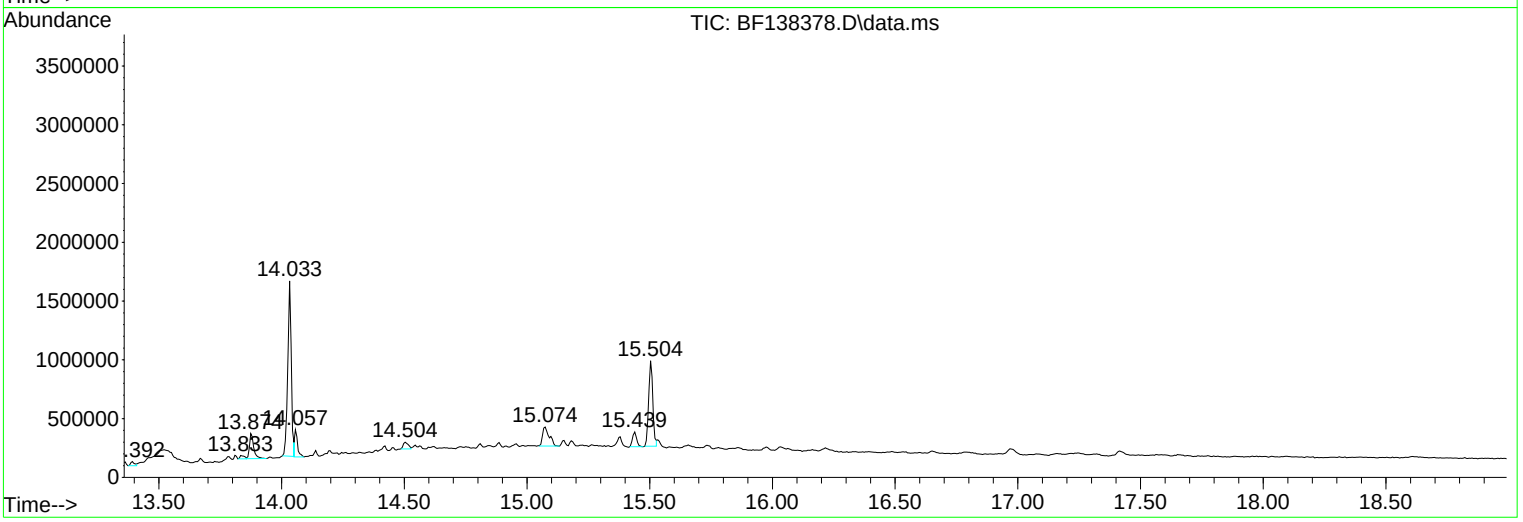
Instrument :
BNA_F
ClientSampleId :
1-W-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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_F\Data\BF062724\
Data File : BF138378.D
Acq On : 27 Jun 2024 21:09
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

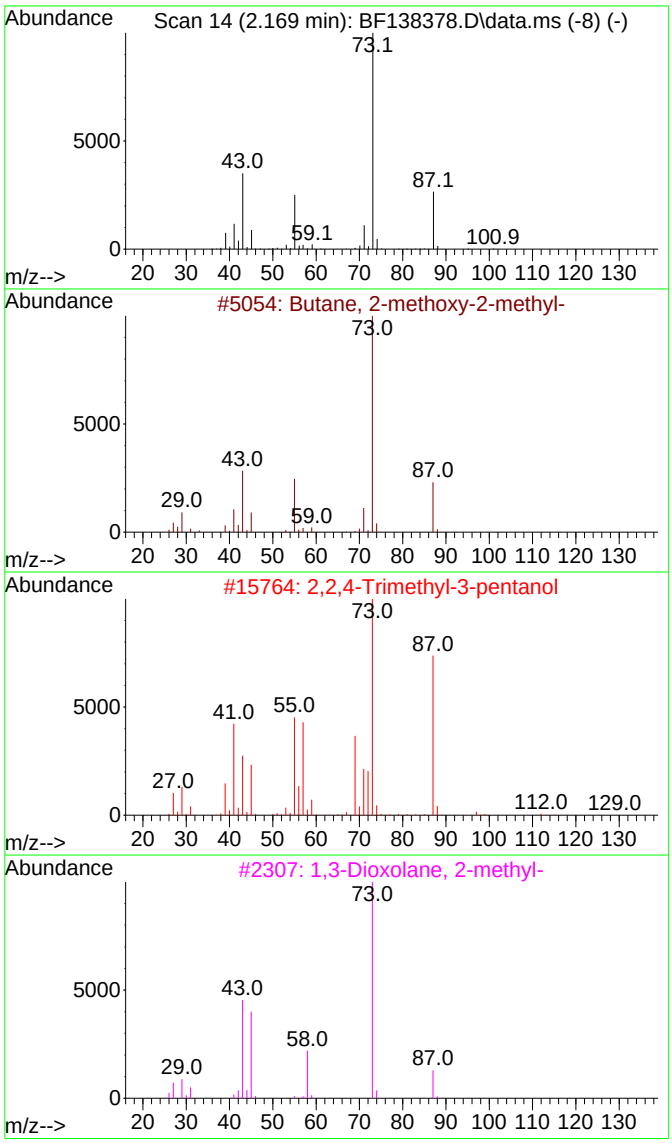
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

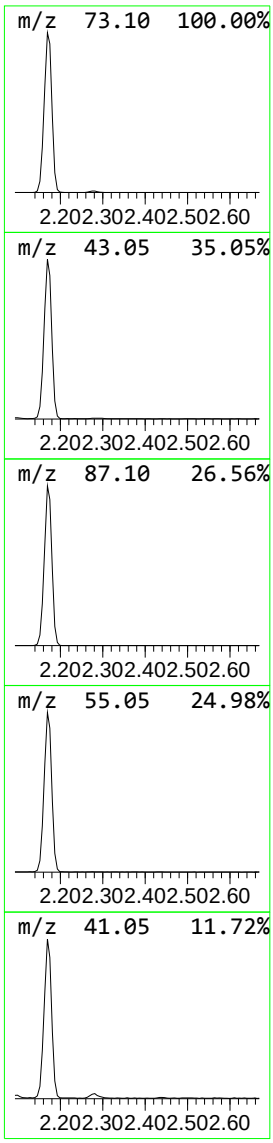
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	35.96 ng	2302830	1,4-Dichlorobenzene-d4	6.881

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138378.D
Acq On : 27 Jun 2024 21:09
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

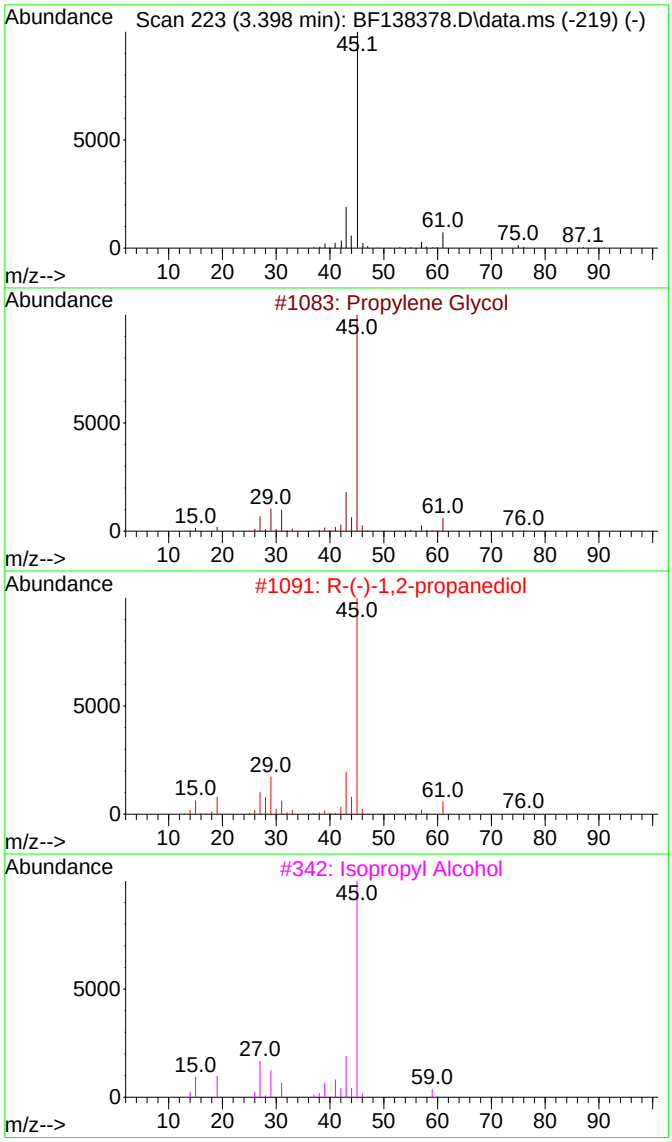
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

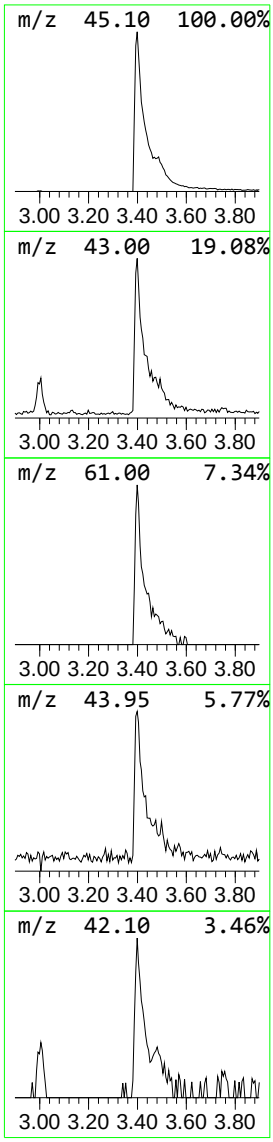
****

Peak Number 2 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.398	2.89 ng	185031	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
5	Methoxyacetic acid, pentyl ester	160	C8H16O3	168920-35-2	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138378.D
Acq On : 27 Jun 2024 21:09
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

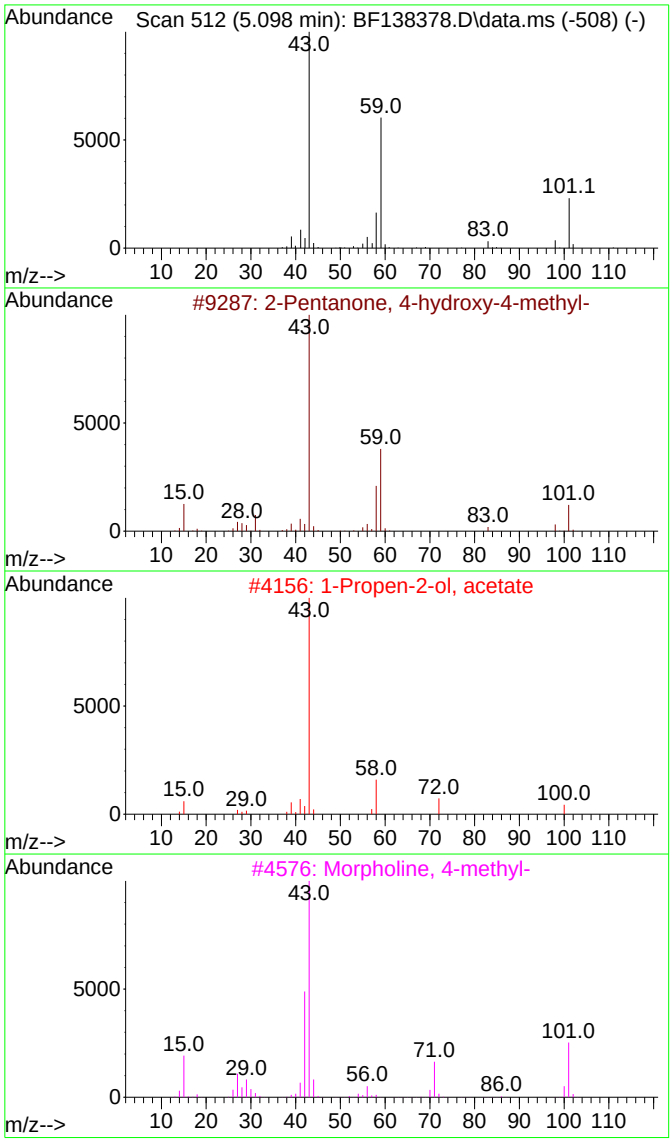
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

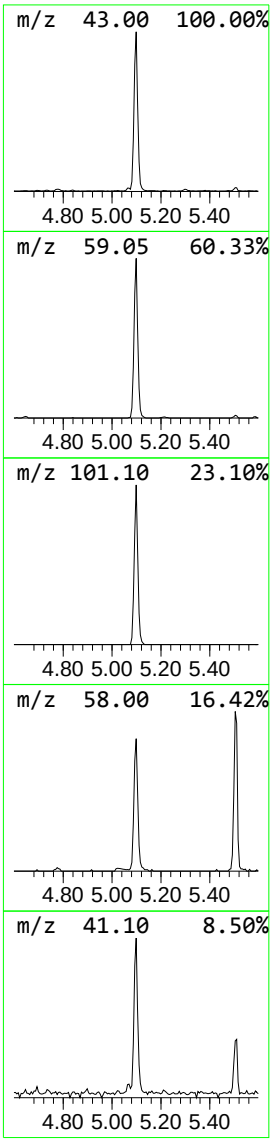
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	3.95 ng	253296	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
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Acq On : 27 Jun 2024 21:09
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

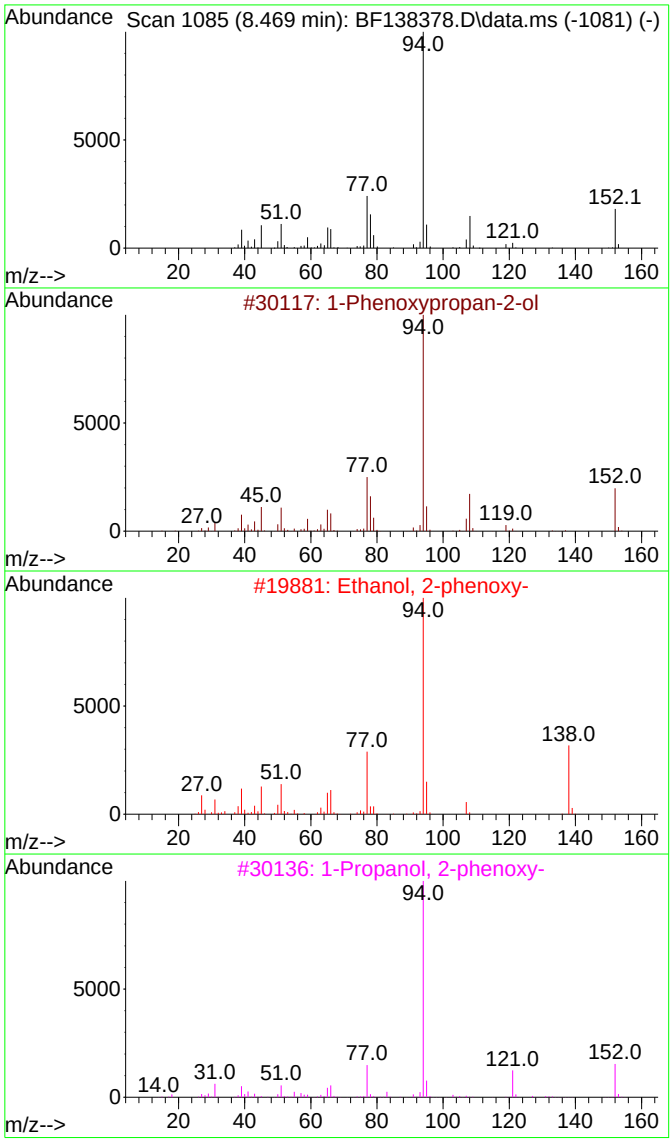
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

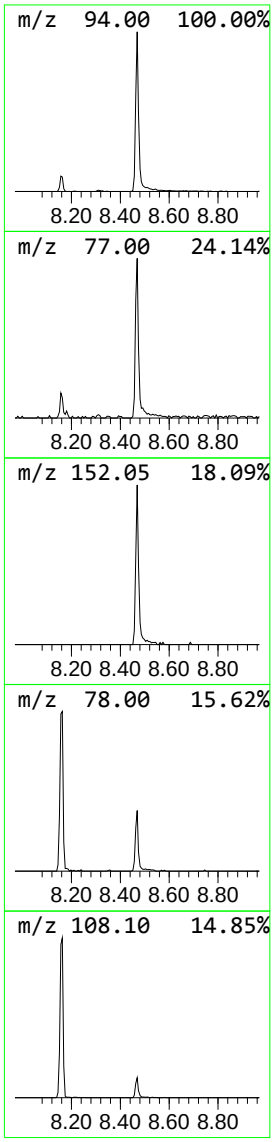
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	2.34 ng	184547	Naphthalene-d8	8.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
5	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138378.D
Acq On : 27 Jun 2024 21:09
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

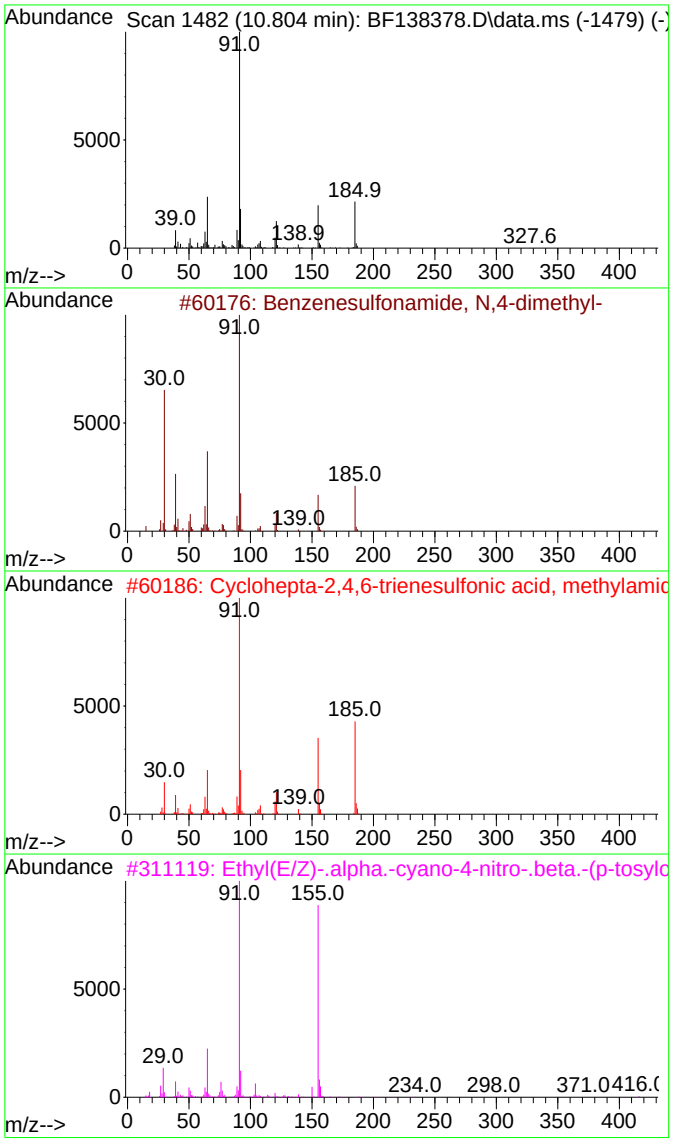
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

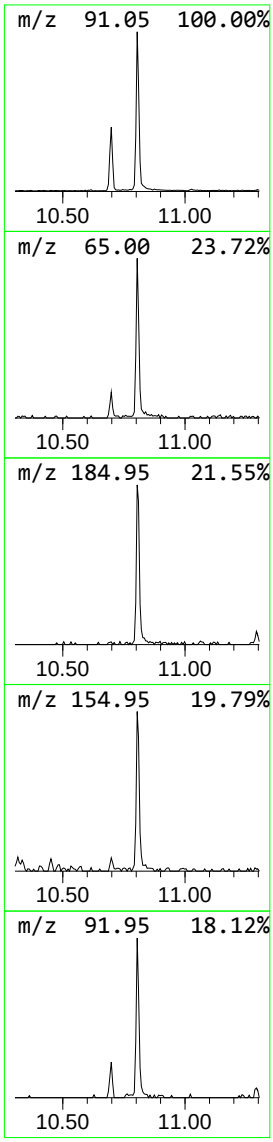
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzenesulfonamide, N,4-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.804	3.14 ng	192299	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	95
2	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	62
3	Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	53
4	p-Toluenesulfonylacetonitrile	195	C9H9NO2S	005697-44-9	47
5	(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	47





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Data File : BF138378.D
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Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

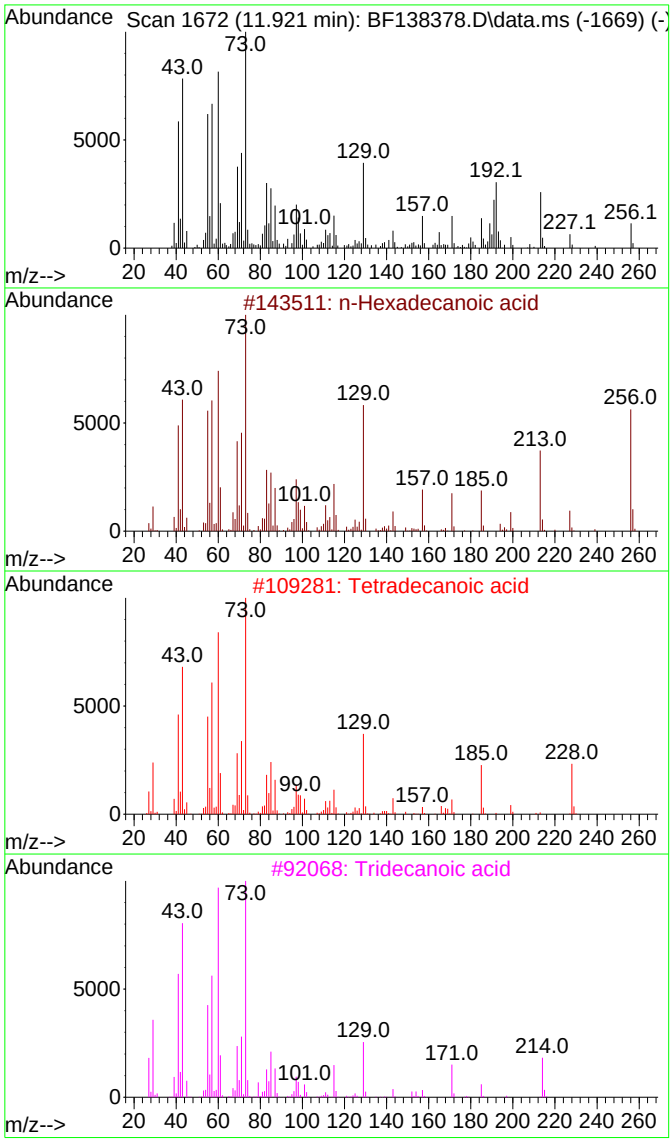
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

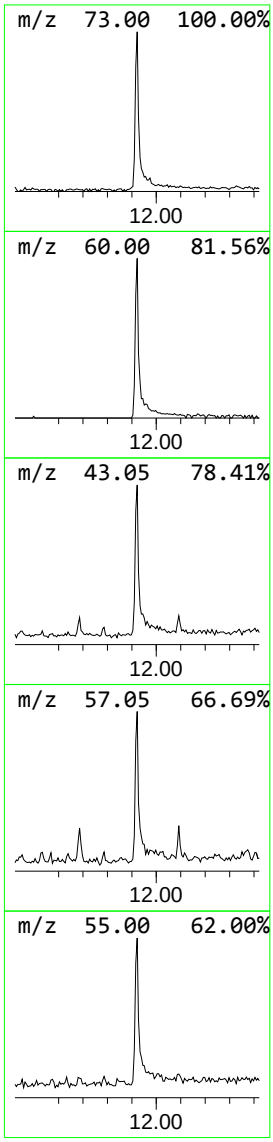
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.12 ng	190827	Phenanthrene-d10	11.398

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	86
4	Undecanoic acid	186	C11H22O2	000112-37-8	76
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	70





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Data File : BF138378.D
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Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

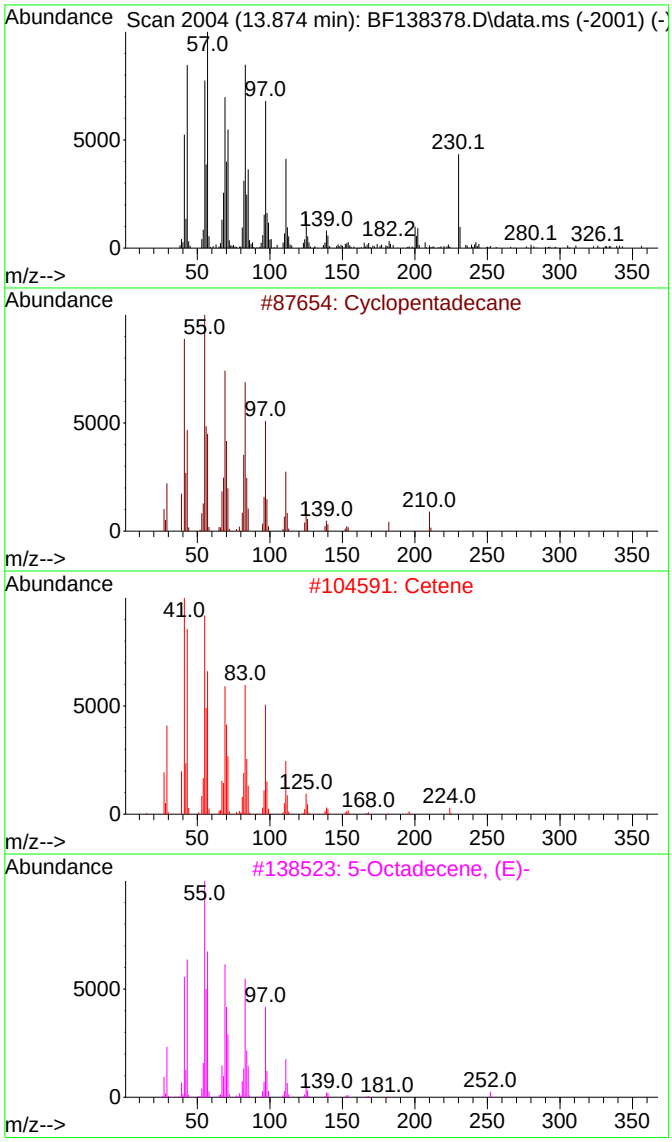
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

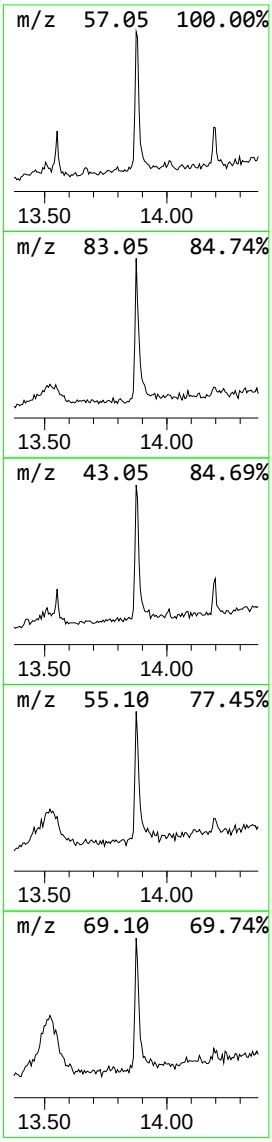
****

Peak Number 7 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.37 ng	253060	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	98
2	Cetene	224	C16H32	000629-73-2	96
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
4	Cyclohexadecane	224	C16H32	000295-65-8	93
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138378.D
Acq On : 27 Jun 2024 21:09
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.169	36.0	ng	2302830	1	6.881	1280910	20.0
Propylene Glycol	3.398	2.9	ng	185031	1	6.881	1280910	20.0
2-Pentanone, 4-...	5.098	4.0	ng	253296	1	6.881	1280910	20.0
1-Phenoxypropan...	8.469	2.3	ng	184547	2	8.163	1579910	20.0
Benzenesulfonam...	10.804	3.1	ng	192299	4	11.398	1224520	20.0
n-Hexadecanoic ...	11.922	3.1	ng	190827	4	11.398	1224520	20.0
Cyclopentadecane	13.874	3.4	ng	253060	5	14.033	1500490	20.0