LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131031.D
Acq On : 05 Nov 2022 21:32
Operator : CG\JU
Sample : N5378-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-20221028-10.5-11.5

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131031.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	12	21	28	rVB	484983	650304	26.95%	3.612%
2	2.322	35	40	46	rVB	52779	66654	2.76%	0.370%
3	5.134	513	518	527	rVB	295697	371162	15.38%	2.061%
4	5.522	579	584	587	rBV	2248136	2345135	97.18%	13.024%
5	6.528	749	755	758	rBV	2336855	2413191	100.00%	13.402%
6	6.898	815	818	822	rBV	608278	516017	21.38%	2.866%
7	7.469	909	915	918	rBV	1481319	1566518	64.91%	8.700%
8	8.087	1016	1020	1032	rBV2	33483	71896	2.98%	0.399%
9	8.187	1032	1037	1040	rBV	772829	657654	27.25%	3.652%
10	9.263	1215	1220	1223	rBV	2749610	2410172	99.87%	13.386%
11	9.945	1331	1336	1339	rBV	925325	736224	30.51%	4.089%
12	10.739	1466	1471	1474	rBV	1825830	1604139	66.47%	8.909%
13	11.439	1586	1590	1593	rBV	881724	729121	30.21%	4.049%
14	11.504	1597	1601	1605	rVB2	46186	47646	1.97%	0.265%
15	12.051	1691	1694	1703	rVB2	31409	43953	1.82%	0.244%
16	12.527	1771	1775	1780	rVB5	17118	26887	1.11%	0.149%
17	12.651	1793	1796	1799	rBV	76634	68993	2.86%	0.383%
18	12.886	1830	1836	1839	rBV	85613	91783	3.80%	0.510%
19	12.916	1839	1841	1849	rVB4	19581	32791	1.36%	0.182%
20	13.027	1856	1860	1863	rBV	2212989	1957620	81.12%	10.872%
21	13.998	2017	2025	2033	rBV5	35611	123409	5.11%	0.685%
22	14.086	2034	2040	2043	rVV	559158	548796	22.74%	3.048%
23	14.110	2043	2044	2051	rVV	55271	40943	1.70%	0.227%
24	14.180	2051	2056	2063	rVV	77079	86075	3.57%	0.478%
25	14.545	2115	2118	2121	rBV2	27723	28848	1.20%	0.160%
26	15.139	2214	2219	2222	rBV	35572	52326	2.17%	0.291%
27	15.457	2269	2273	2279	rVB	19657	27007	1.12%	0.150%
28	15.516	2279	2283	2289	rBV	39040	51758	2.14%	0.287%
29	15.586	2290	2295	2303	rVV	327375	420832	17.44%	2.337%
30	16.063	2371	2376	2382	rVB	24862	33978	1.41%	0.189%
31	16.586	2460	2465	2472	rBV3	24853	49821	2.06%	0.277%
32	17.098	2546	2552	2561	rVB3	13759	31483	1.30%	0.175%
33	17.210	2564	2571	2577	rBV4	16810	34905	1.45%	0.194%
34	17.557	2623	2630	2640	rBV2	12032	32014	1.33%	0.178%
35	17.945	2688	2696	2702	rVB10	12216	35643	1.48%	0.198%

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Data File : BF131031.D
Acq On : 05 Nov 2022 21:32
Operator : CG\JU
Sample : N5378-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-20221028-10.5-11.5

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

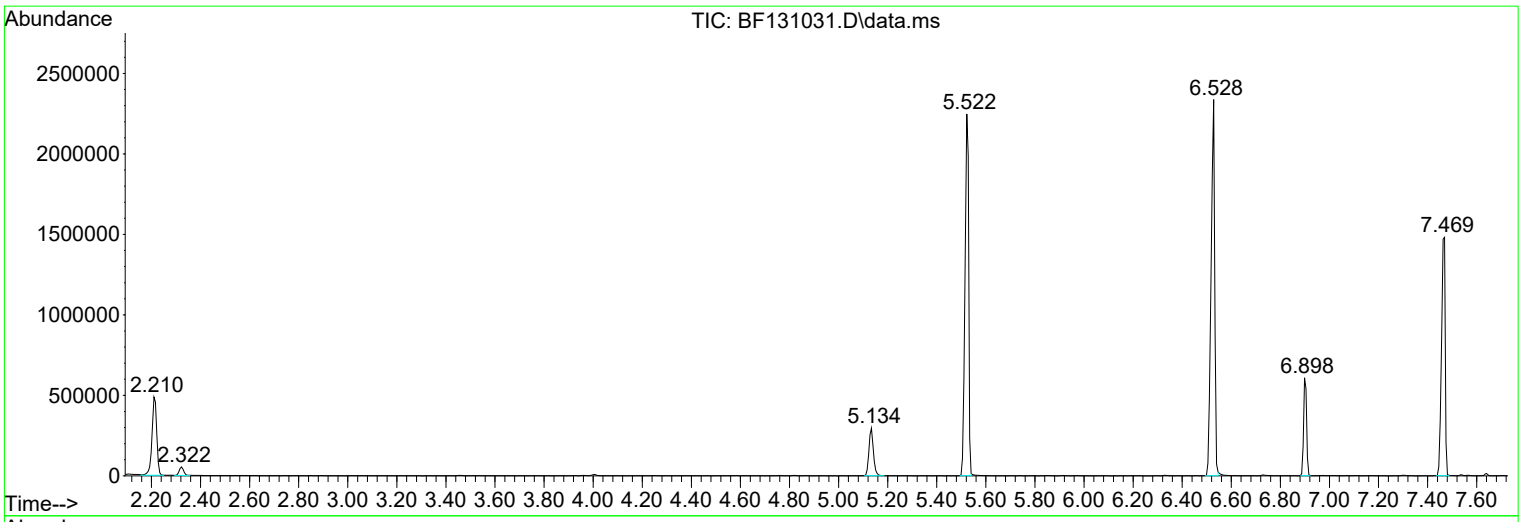
Sum of corrected areas: 18005698

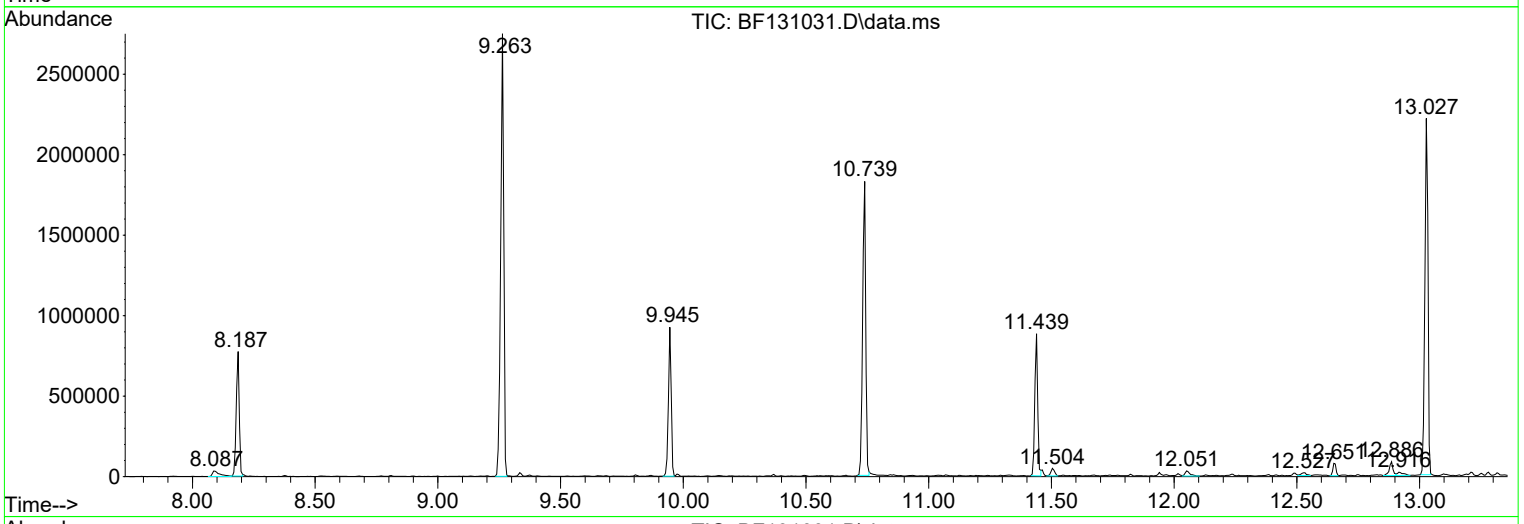
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131031.D
Acq On : 05 Nov 2022 21:32
Operator : CG\JU
Sample : N5378-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

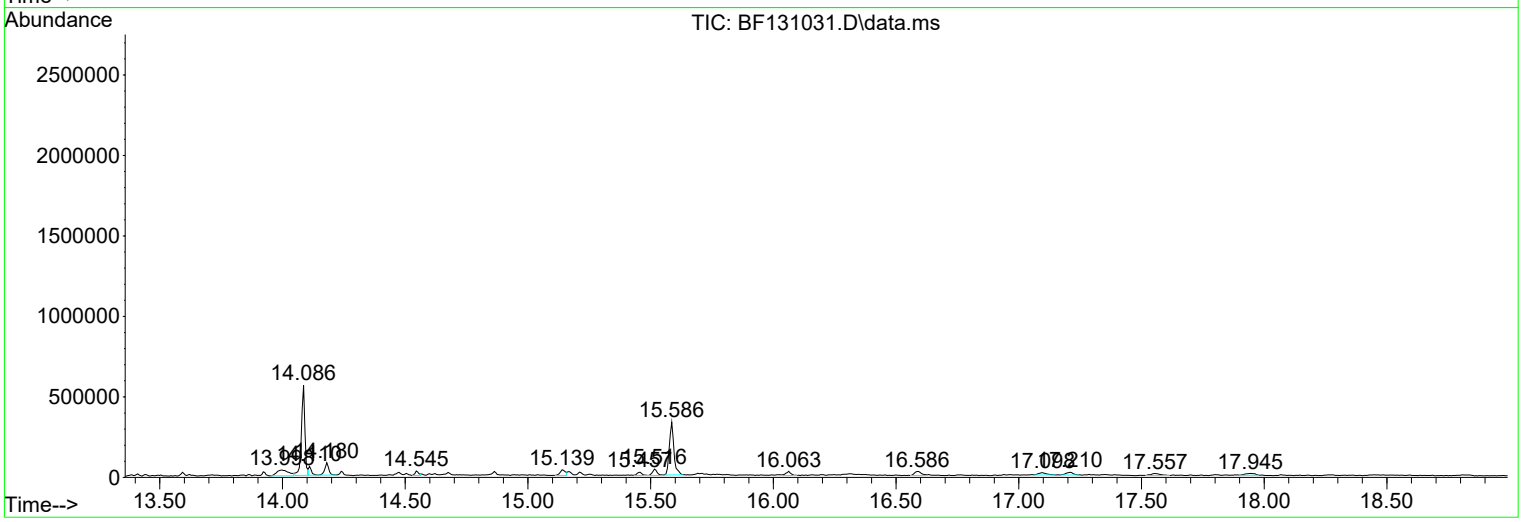
Instrument :
BNA_F
ClientSampleId :
SB-16-20221028-10.5-11.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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Data File : BF131031.D
Acq On : 05 Nov 2022 21:32
Operator : CG\JU
Sample : N5378-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-16-20221028-10.5-11.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

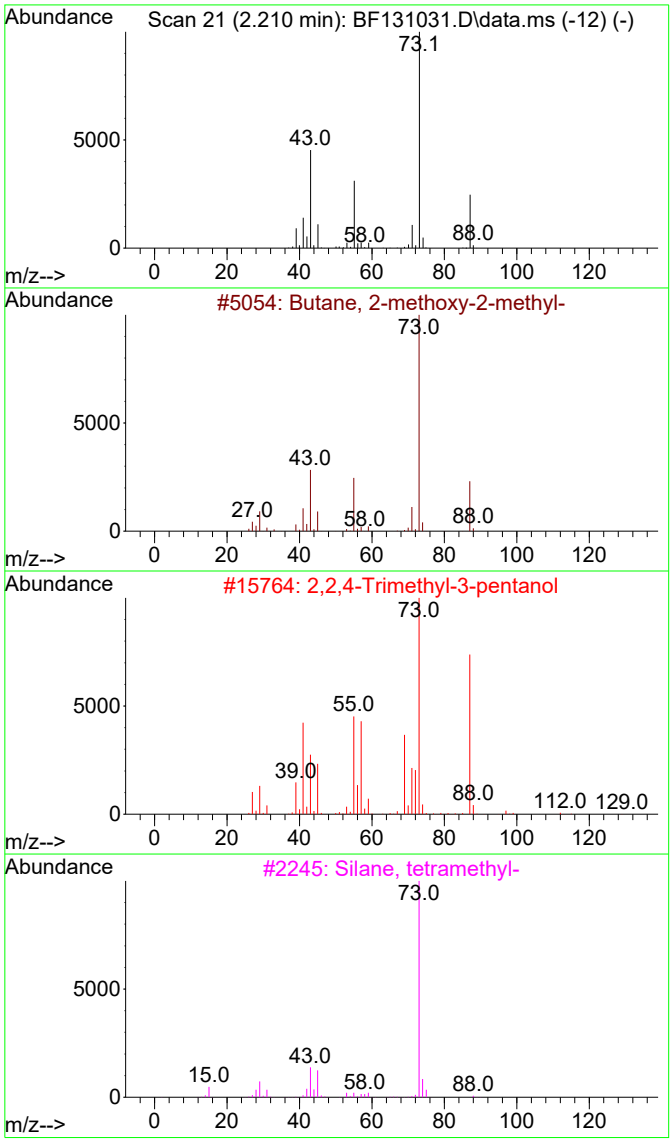
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

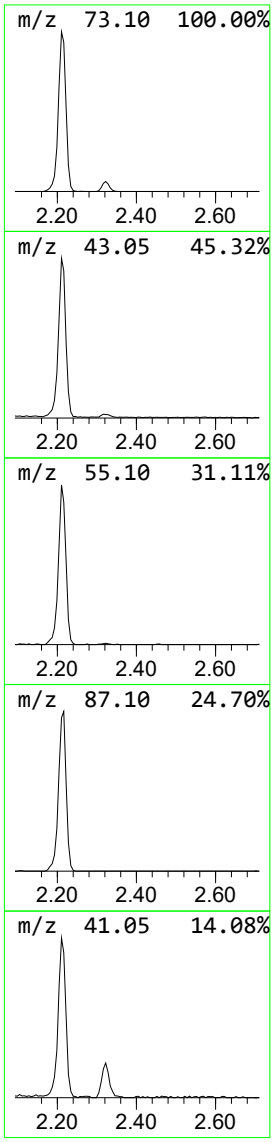
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.210	25.20 ng	650304	1,4-Dichlorobenzene-d4	6.898

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	38
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
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Operator : CG\JU
Sample : N5378-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-20221028-10.5-11.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

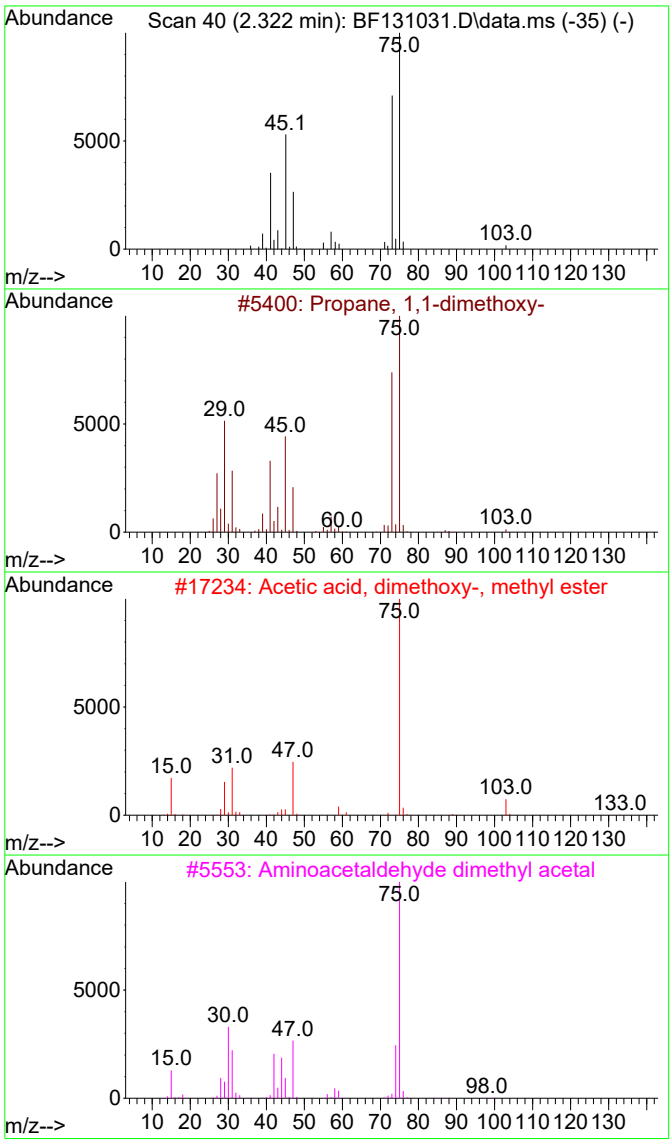
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

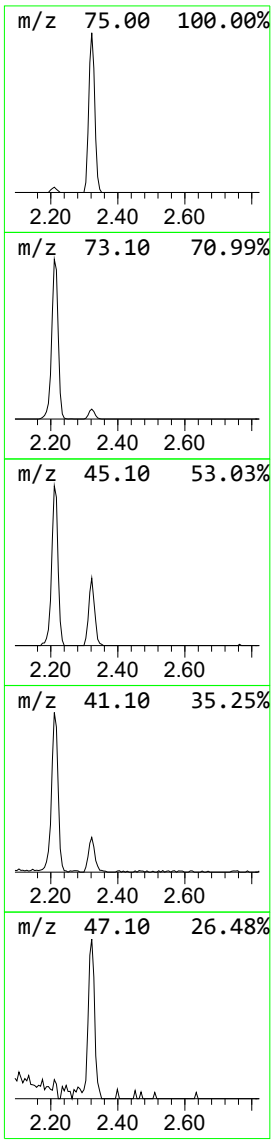
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.322	2.58 ng	66654	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	40
3	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	33
4	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
5	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131031.D
Acq On : 05 Nov 2022 21:32
Operator : CG\JU
Sample : N5378-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-20221028-10.5-11.5

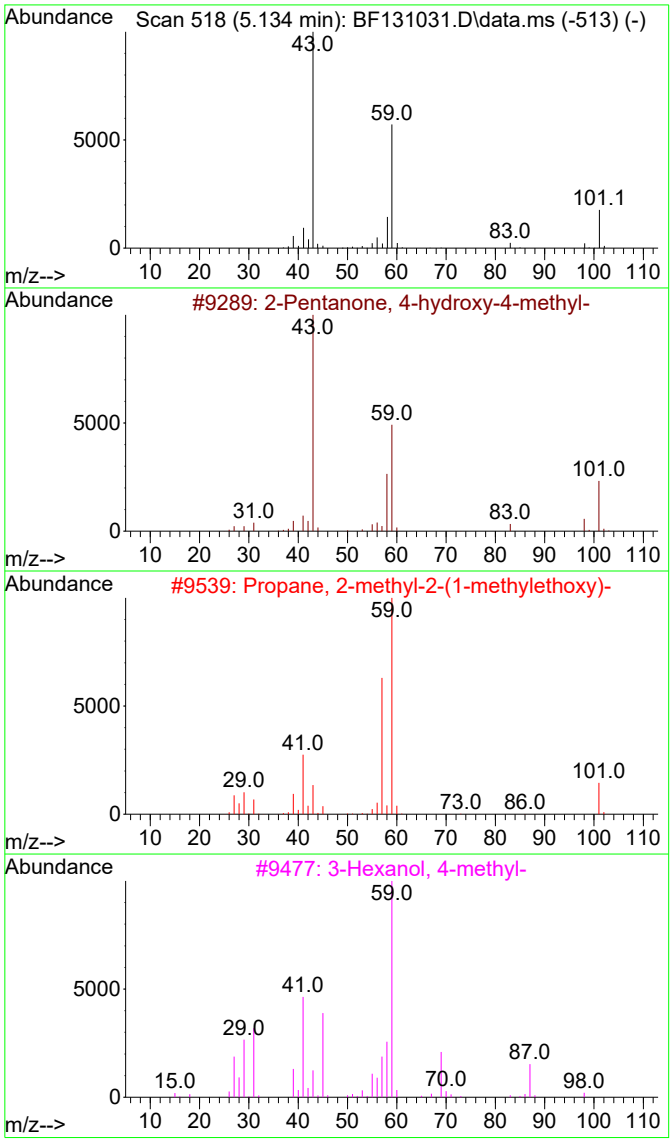
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

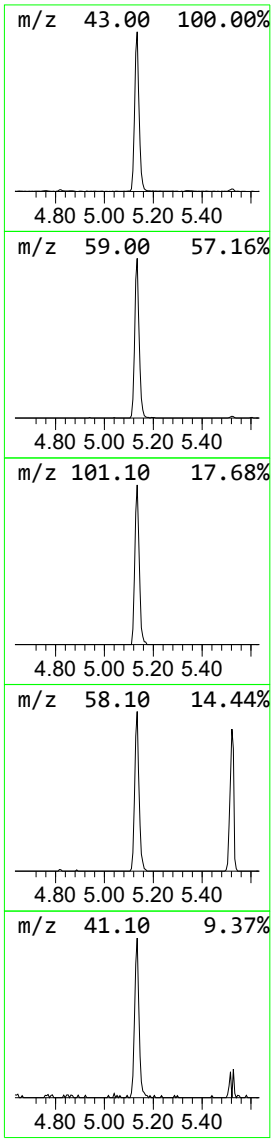
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	14.39 ng	371162	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
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Acq On : 05 Nov 2022 21:32
Operator : CG\JU
Sample : N5378-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-20221028-10.5-11.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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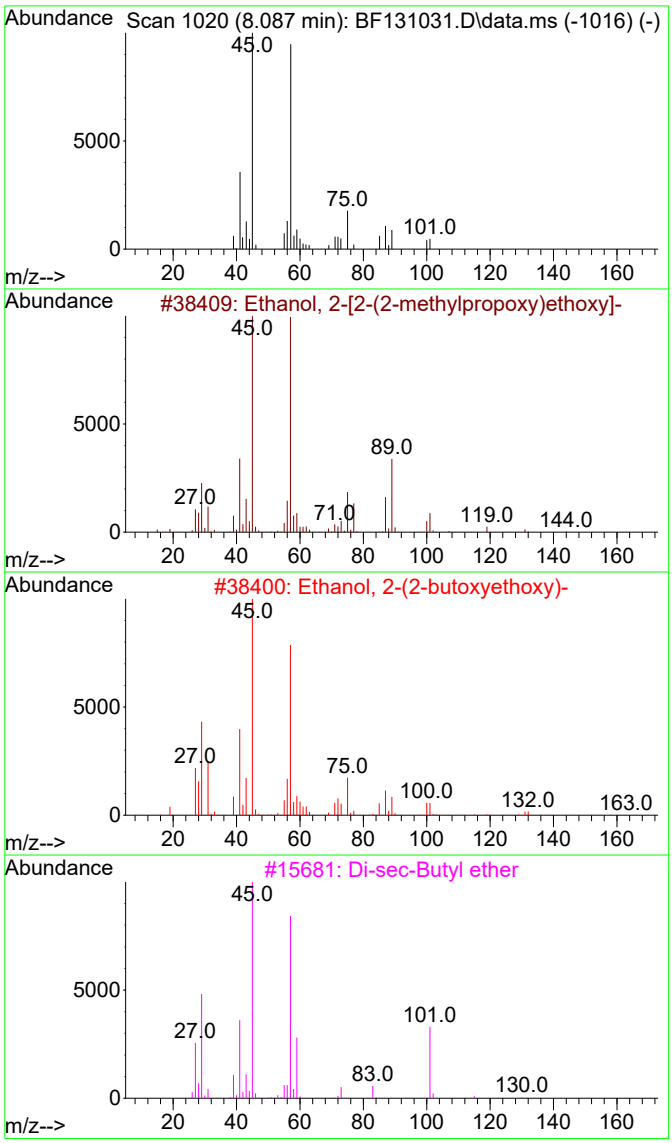
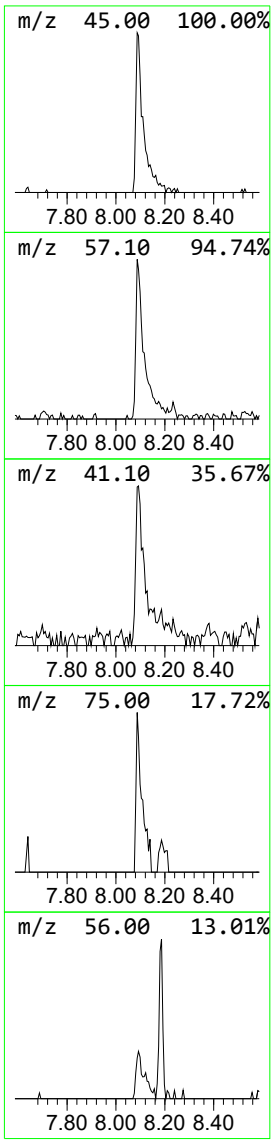
Peak Number 4 Ethanol, 2-[2-(2-methylprop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.087	2.19 ng	71896	Naphthalene-d8	8.187

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
3	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
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Sample : N5378-02
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-20221028-10.5-11.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

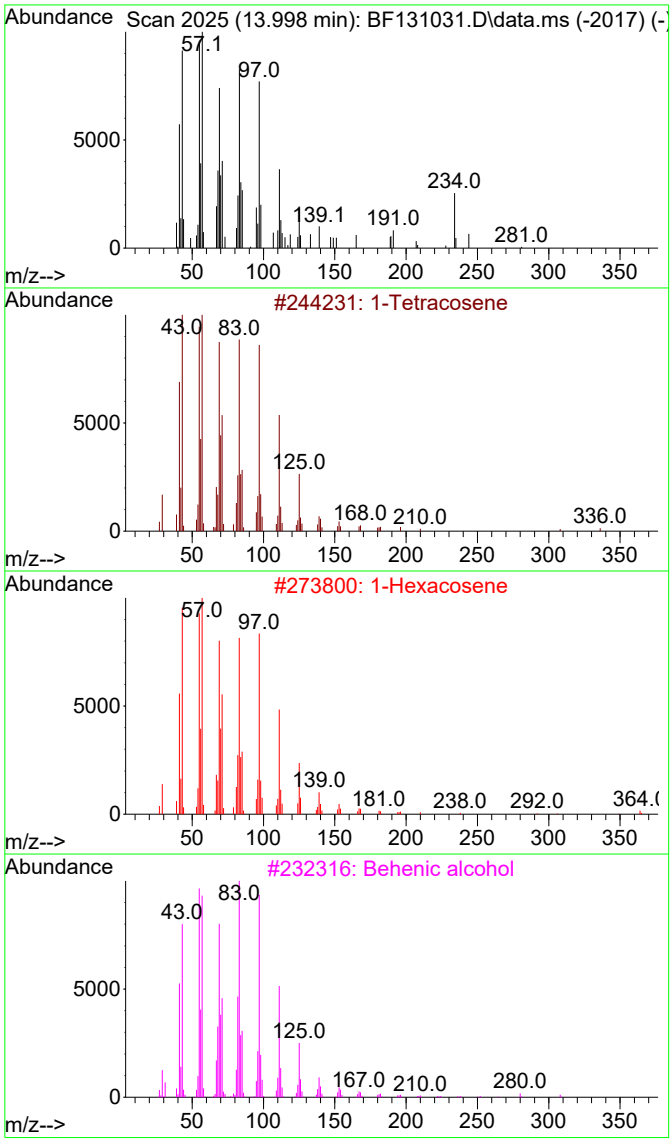
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

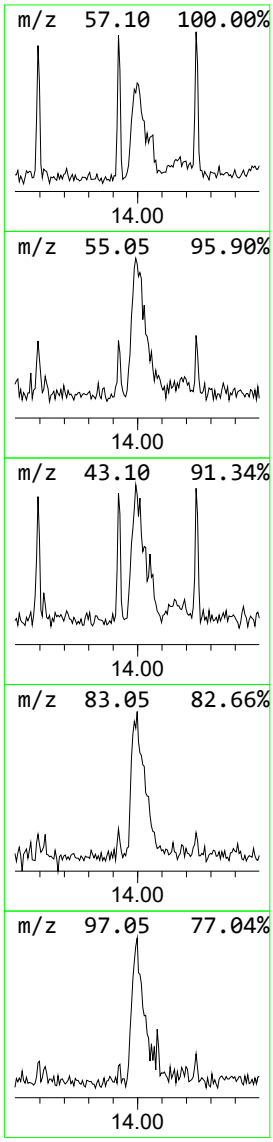
****

Peak Number 5 1-Tetracosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	4.50 ng	123409	Chrysene-d12	14.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	93
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
5	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131031.D
Acq On : 05 Nov 2022 21:32
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-20221028-10.5-11.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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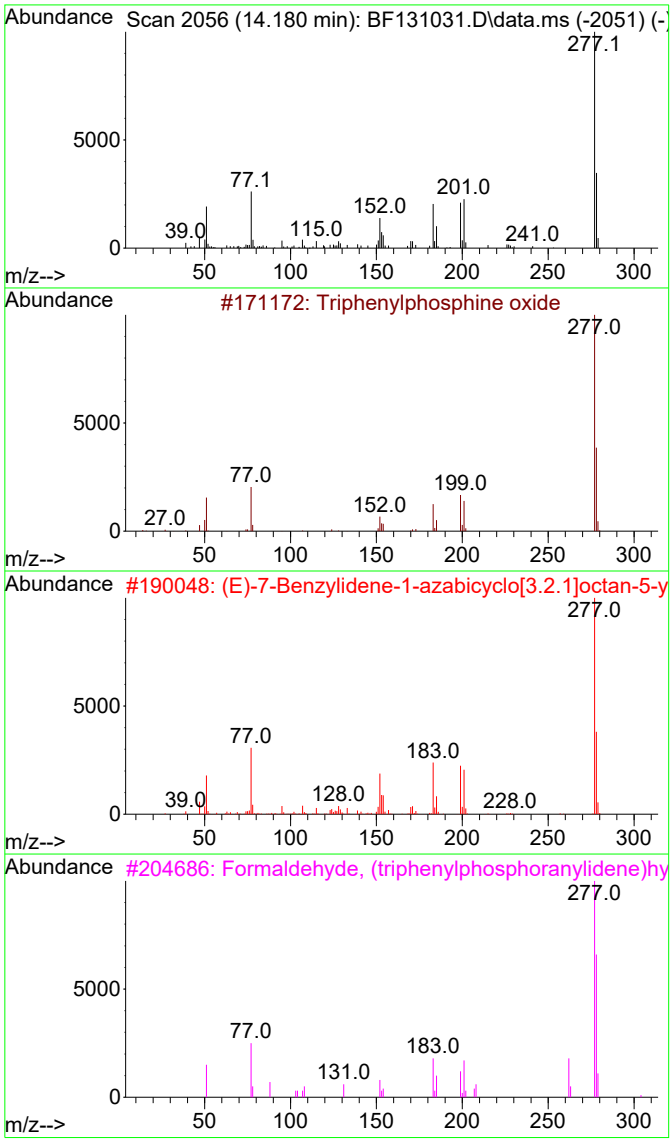
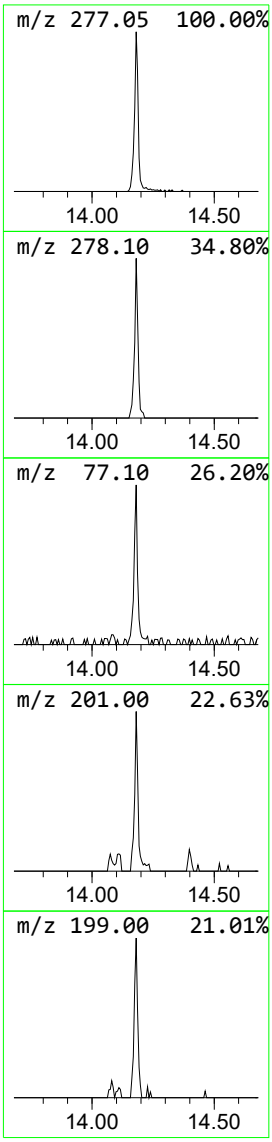
Peak Number 6 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.180	3.14 ng	86075	Chrysene-d12	14.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	87
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	32
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	12





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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

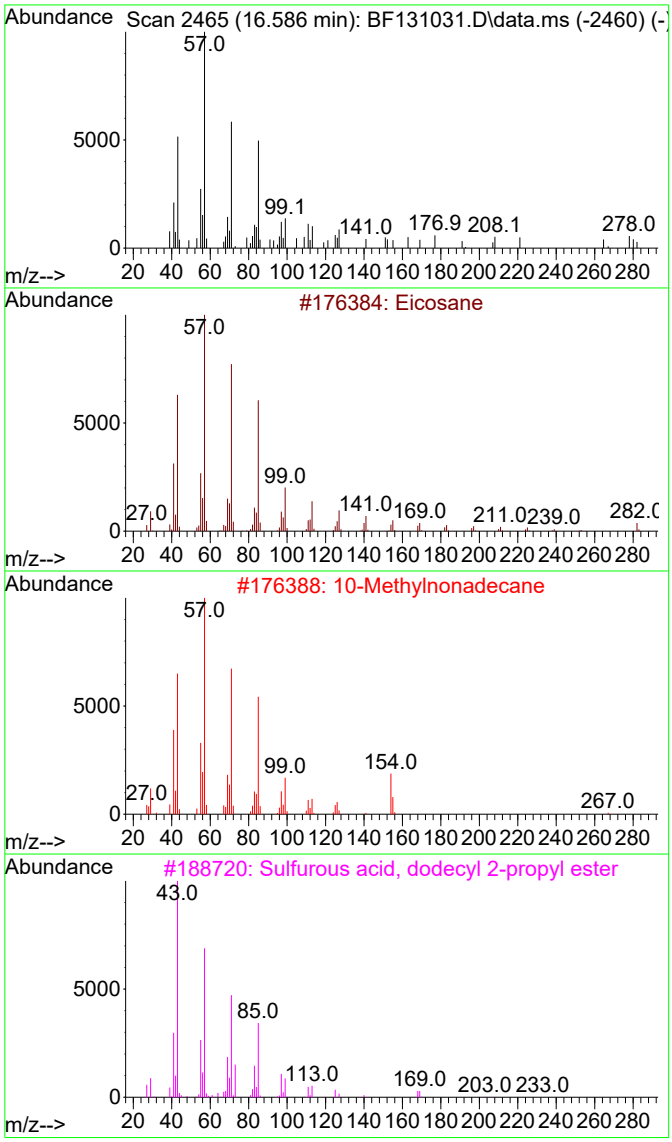
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

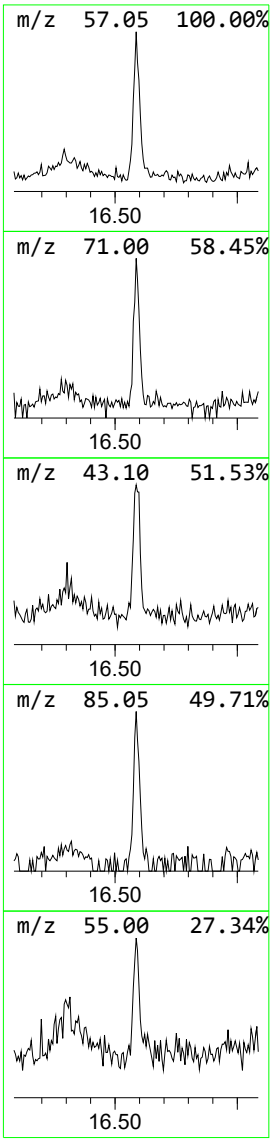
****

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.586	2.37 ng	49821	Perylene-d12	15.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	10-Methylnonadecane	282	C20H42	056862-62-5	80
3	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	80
4	Hexacosane	366	C26H54	000630-01-3	74
5	Heneicosane	296	C21H44	000629-94-7	74





Tentatively Identified Compound (LSC) summary

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Data File : BF131031.D
Acq On : 05 Nov 2022 21:32
Operator : CG\JU
Sample : N5378-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-20221028-10.5-11.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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...	2.210	25.2	ng	650304	1	6.898	516017	20.0
Propane, 1,1-di...	2.322	2.6	ng	66654	1	6.898	516017	20.0
2-Pentanone, 4-...	5.134	14.4	ng	371162	1	6.898	516017	20.0
Ethanol, 2-[2-(...	8.087	2.2	ng	71896	2	8.187	657654	20.0
1-Tetracosene	13.998	4.5	ng	123409	5	14.086	548796	20.0
Triphenylphosph...	14.180	3.1	ng	86075	5	14.086	548796	20.0
Eicosane	16.586	2.4	ng	49821	6	15.586	420832	20.0