LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111220\
Data File : BP003940.D
Acq On : 12 Nov 2020 15:59
Operator : CG/JU
Sample : L4719-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-3-S

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\8270-BP110320.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003940.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	3	7	21	rVB	2703777	2982449	63.58%	8.630%
2	3.087	28	34	45	rVV	124002	250276	5.34%	0.724%
3	3.175	45	49	60	rVB	357853	440447	9.39%	1.275%
4	5.805	489	496	505	rBV	2032810	2987885	63.70%	8.646%
5	7.452	768	776	793	rBV	1899068	3072118	65.50%	8.890%
6	7.852	837	844	852	rVB	56117	85680	1.83%	0.248%
7	8.281	909	917	924	rBV	554892	856827	18.27%	2.479%
8	9.446	1107	1115	1125	rBV	1185621	1982163	42.26%	5.736%
9	11.110	1391	1398	1405	rBV	651114	1105914	23.58%	3.200%
10	13.528	1801	1809	1825	rBV	2507569	3817610	81.39%	11.047%
11	14.328	1939	1945	1955	rBV	426617	604325	12.88%	1.749%
12	14.628	1991	1996	2000	rBV2	29716	53667	1.14%	0.155%
13	14.692	2001	2007	2020	rVB	52755	137371	2.93%	0.398%
14	14.904	2037	2043	2051	rBV	941723	1362599	29.05%	3.943%
15	16.386	2288	2295	2312	rBV	1908566	2796001	59.61%	8.091%
16	16.880	2375	2379	2390	rBV3	21647	49613	1.06%	0.144%
17	16.998	2395	2399	2411	rVB7	34080	82682	1.76%	0.239%
18	17.639	2501	2508	2513	rBV	1047052	1548235	33.01%	4.480%
19	18.475	2646	2650	2656	rBV4	57342	99336	2.12%	0.287%
20	18.739	2692	2695	2699	rVV2	67780	104867	2.24%	0.303%
21	18.780	2699	2702	2712	rVB2	75795	137443	2.93%	0.398%
22	19.227	2774	2778	2783	rBV	87311	107938	2.30%	0.312%
23	19.610	2840	2843	2849	rVB	58875	73004	1.56%	0.211%
24	19.733	2855	2864	2876	rVB4	133782	527155	11.24%	1.525%
25	19.957	2899	2902	2911	rVB	116782	203035	4.33%	0.588%
26	20.133	2927	2932	2938	rBV	3903913	4690566	100.00%	13.573%
27	20.868	3054	3057	3062	rBV2	48507	73553	1.57%	0.213%
28	20.998	3076	3079	3084	rBV	108423	122245	2.61%	0.354%
29	21.110	3090	3098	3108	rVB4	136419	453954	9.68%	1.314%
30	21.321	3130	3134	3143	rVB2	388805	501955	10.70%	1.453%
31	21.392	3143	3146	3150	rBV	110502	118602	2.53%	0.343%
32	21.668	3188	3193	3198	rBV	1145276	1499443	31.97%	4.339%
33	24.157	3609	3616	3622	rVB	805165	1628798	34.72%	4.713%

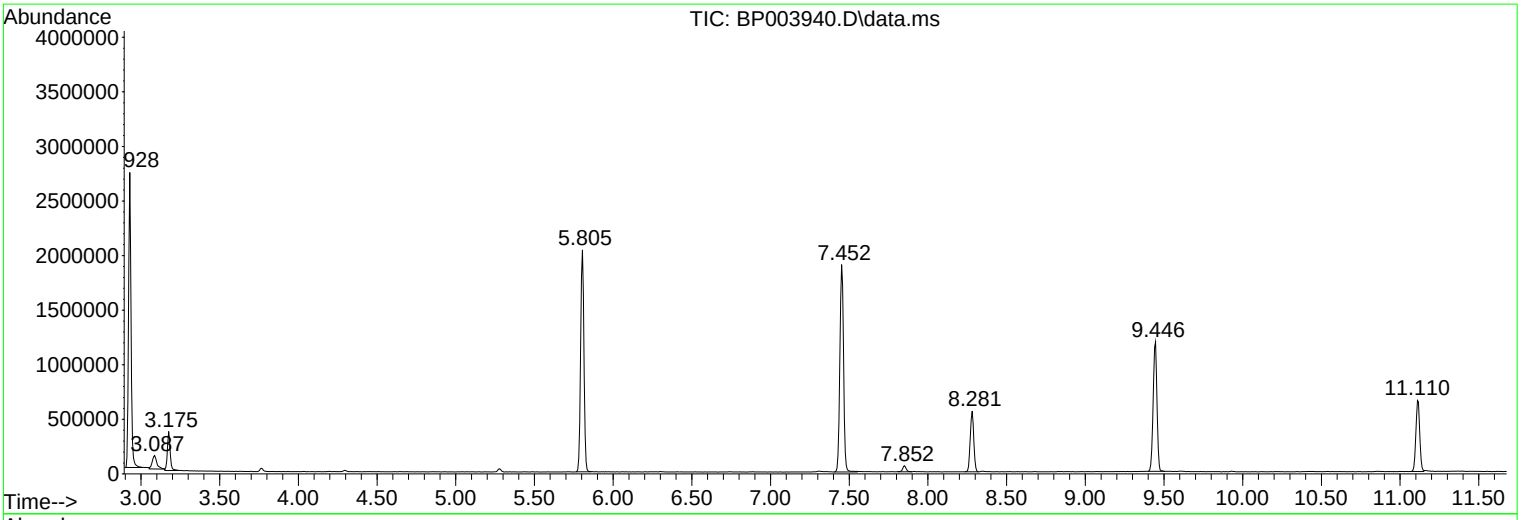
Sum of corrected areas: 34557756

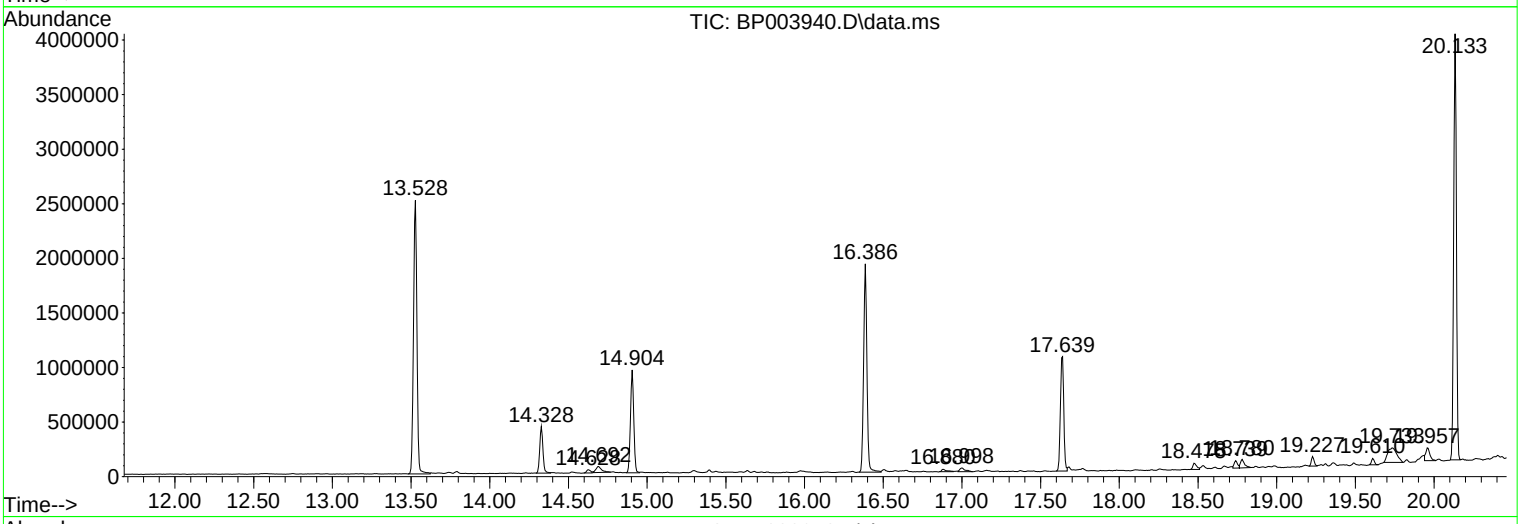
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111220\
Data File : BP003940.D
Acq On : 12 Nov 2020 15:59
Operator : CG/JU
Sample : L4719-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

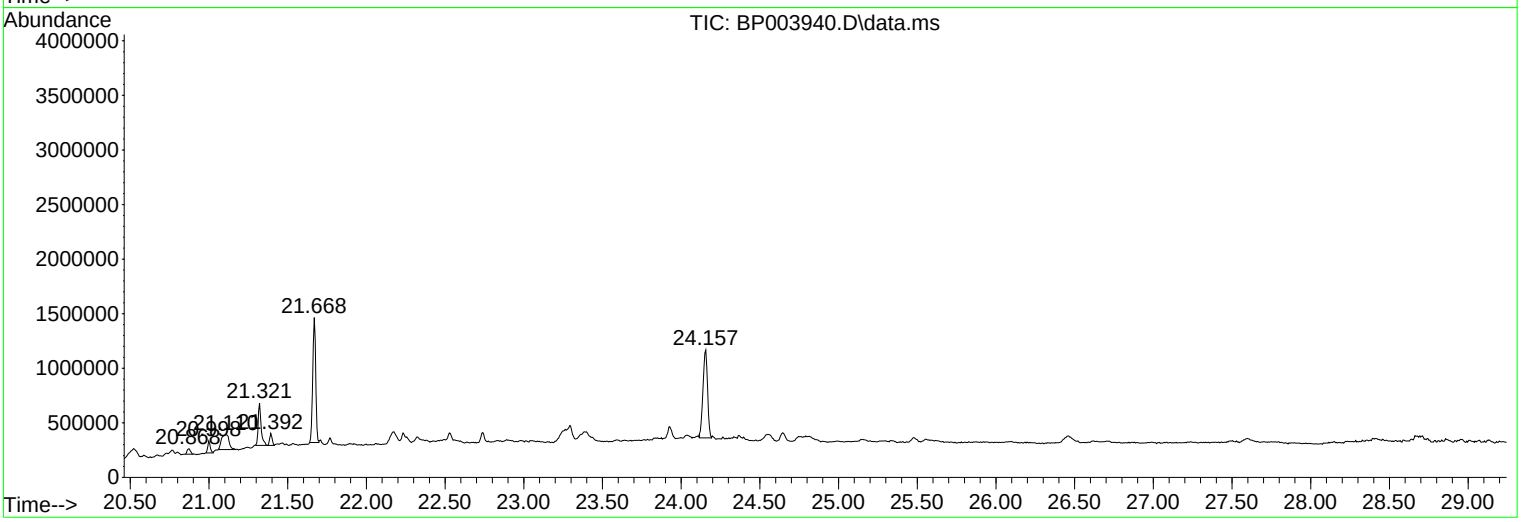
Instrument :
BNA_P
ClientSampleId :
TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111220\
Data File : BP003940.D
Acq On : 12 Nov 2020 15:59
Operator : CG/JU
Sample : L4719-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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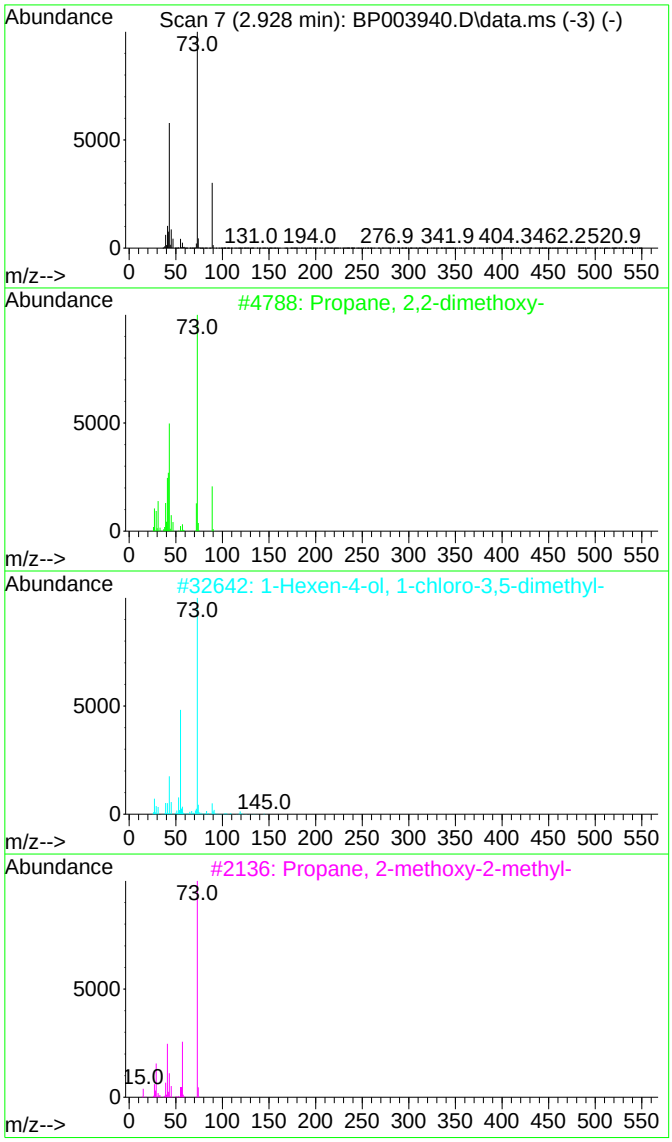
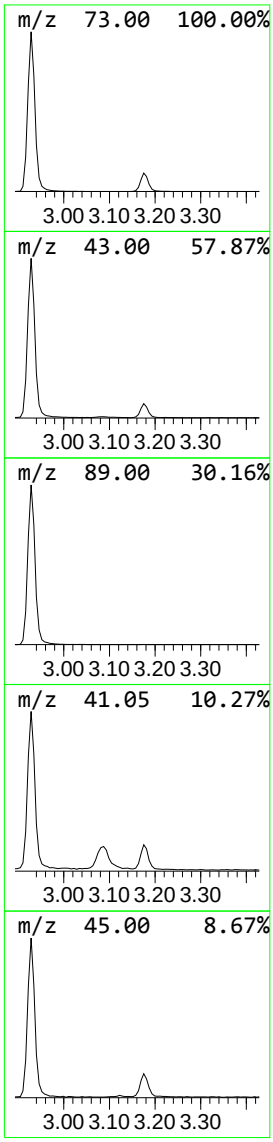
Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.928	69.62 ng	2982450	1,4-Dichlorobenzene-d4	8.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
5	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111220\
Data File : BP003940.D
Acq On : 12 Nov 2020 15:59
Operator : CG/JU
Sample : L4719-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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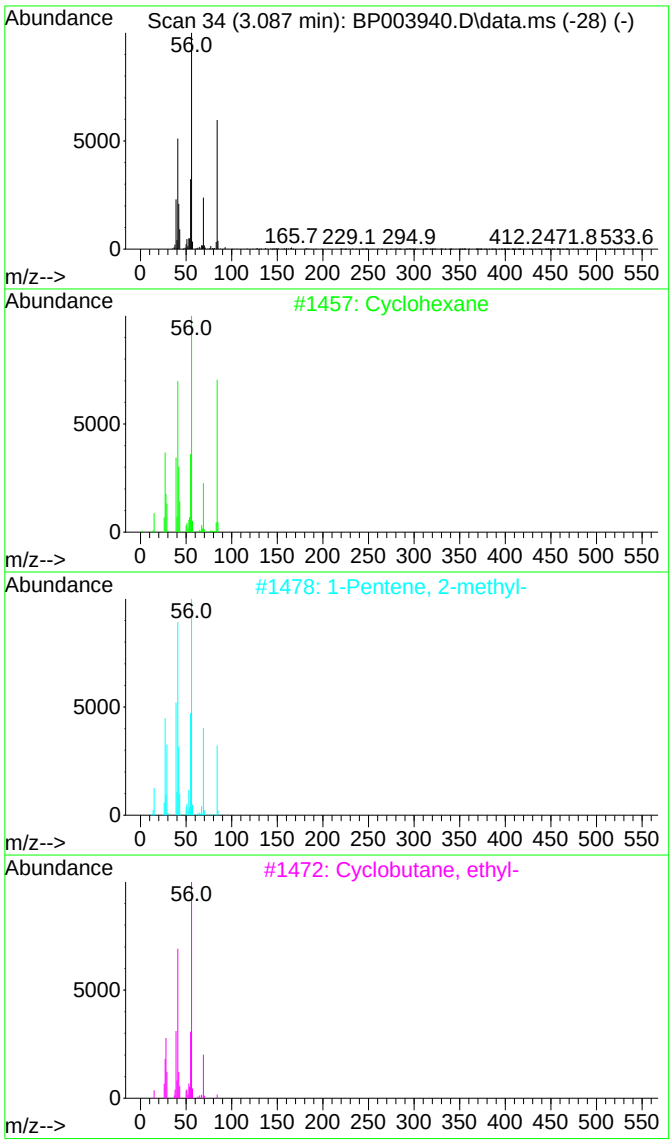
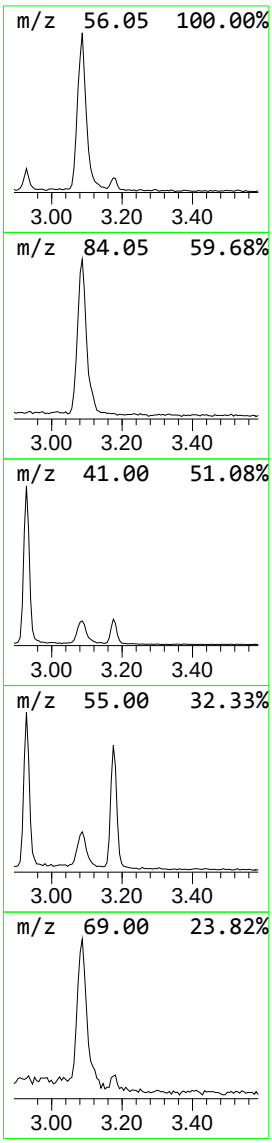
Peak Number 2 Cyclohexane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	5.84 ng	250276	1,4-Dichlorobenzene-d4	8.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	43
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	42
5	Cyclobutane	56	C4H8	000287-23-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111220\
Data File : BP003940.D
Acq On : 12 Nov 2020 15:59
Operator : CG/JU
Sample : L4719-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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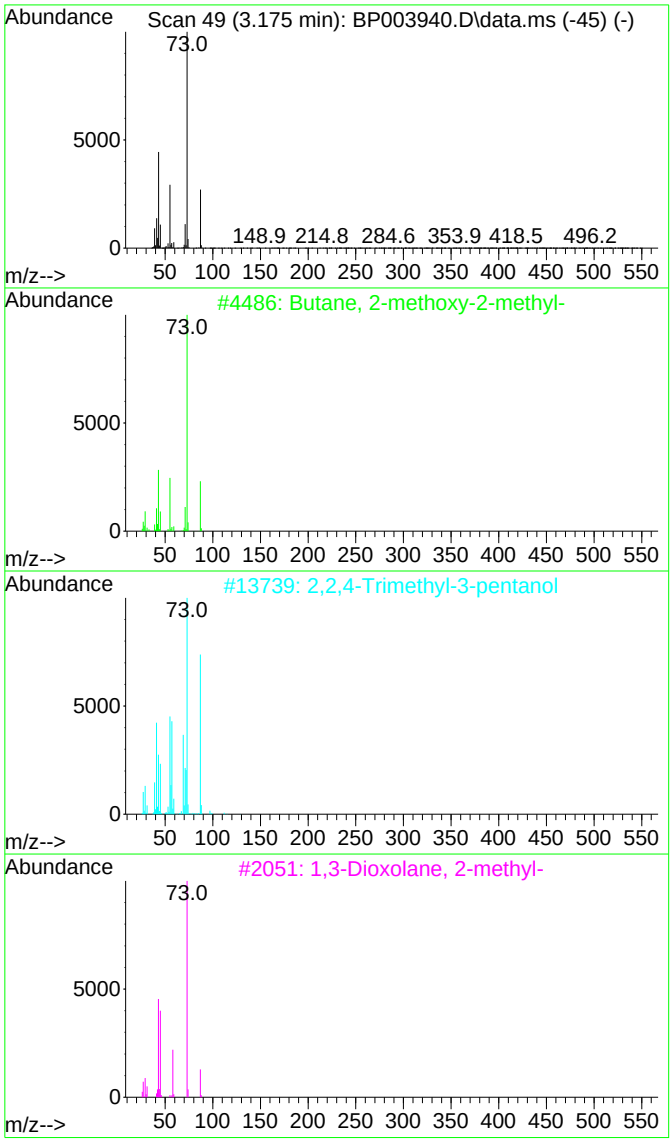
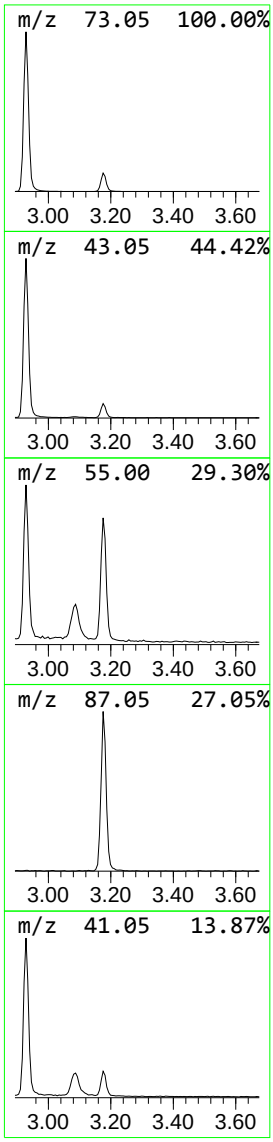
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.175	10.28 ng	440447	1,4-Dichlorobenzene-d4	8.281

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111220\
Data File : BP003940.D
Acq On : 12 Nov 2020 15:59
Operator : CG/JU
Sample : L4719-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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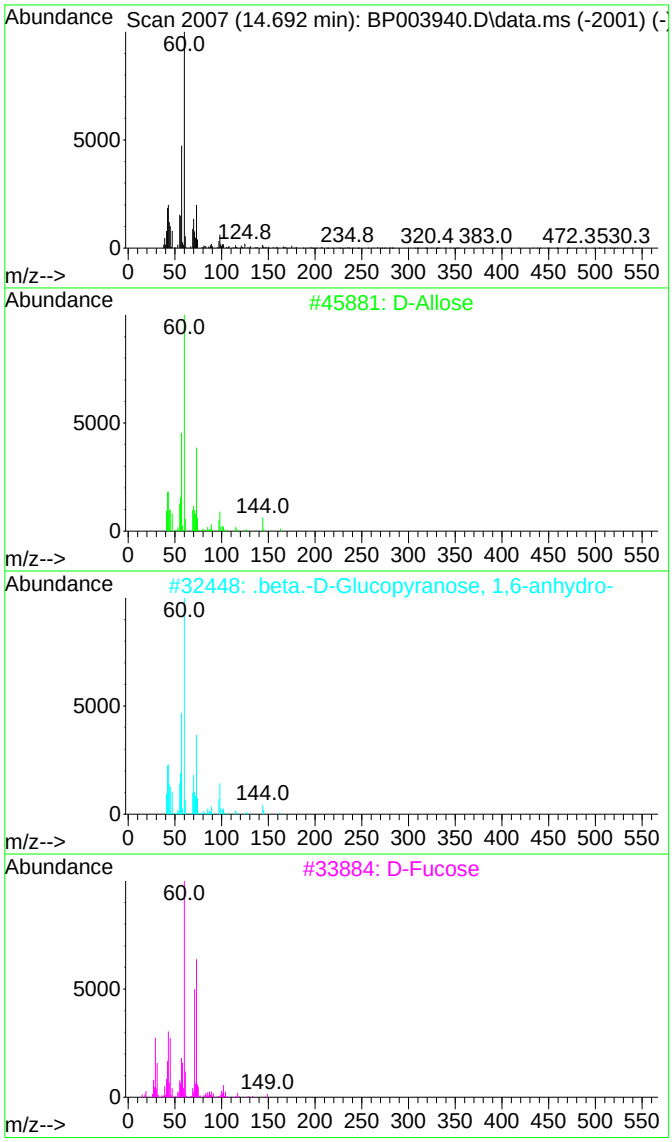
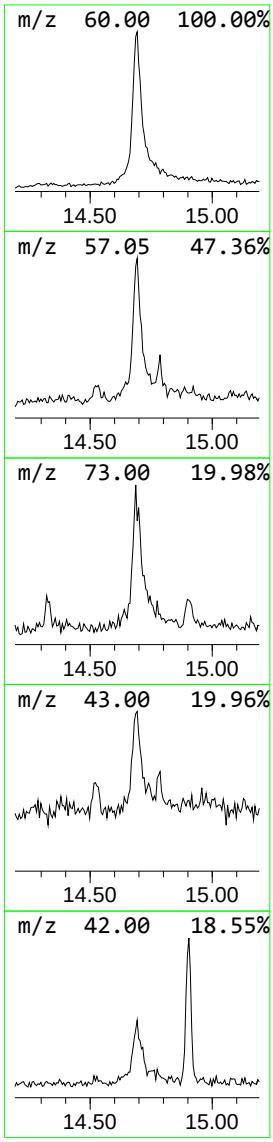
Peak Number 4 D-Allose Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.692	2.02 ng	137371	Acenaphthene-d10	14.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Allose	180	C6H12O6	002595-97-3	83
2	.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	60
3	D-Fucose	164	C6H12O5	003615-37-0	45
4	Hexanoic acid	116	C6H12O2	000142-62-1	45
5	3,4-Altrosan	162	C6H10O5	1000129-76-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111220\
Data File : BP003940.D
Acq On : 12 Nov 2020 15:59
Operator : CG/JU
Sample : L4719-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

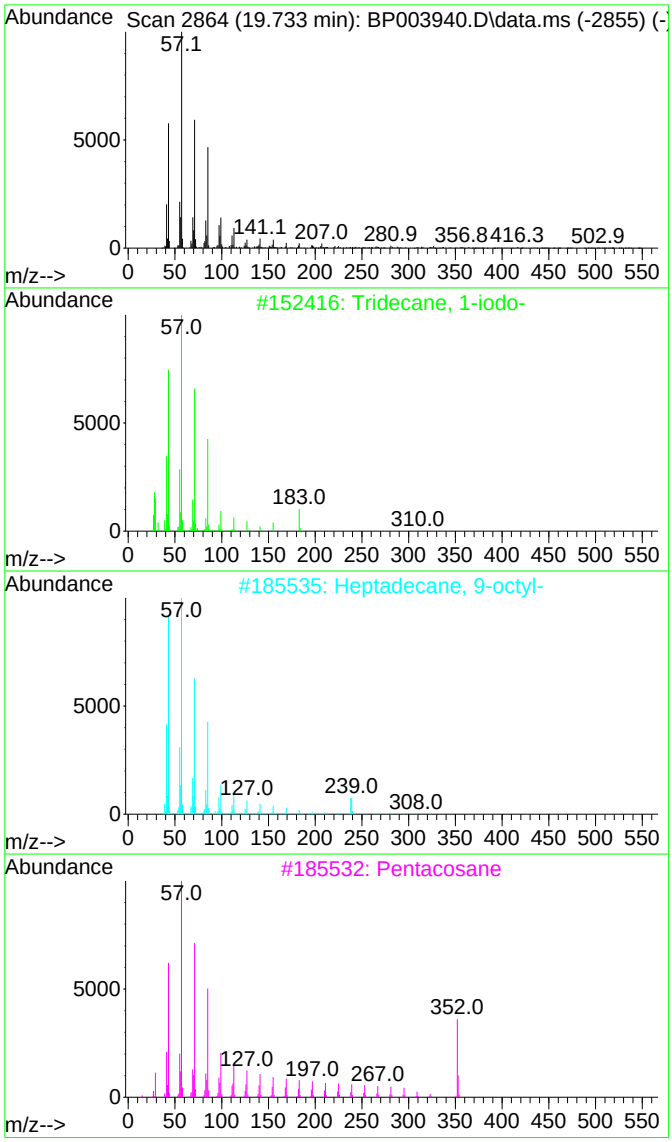
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

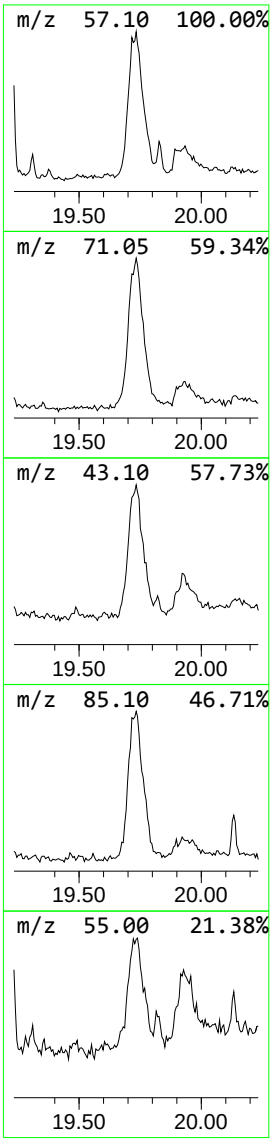
****

Peak Number 5 Tridecane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.733	7.03 ng	527155	Chrysene-d12	21.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	94
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
3	Pentacosane	352	C25H52	000629-99-2	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Docosane, 11-decyl-	451	C32H66	055401-55-3	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111220\
Data File : BP003940.D
Acq On : 12 Nov 2020 15:59
Operator : CG/JU
Sample : L4719-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

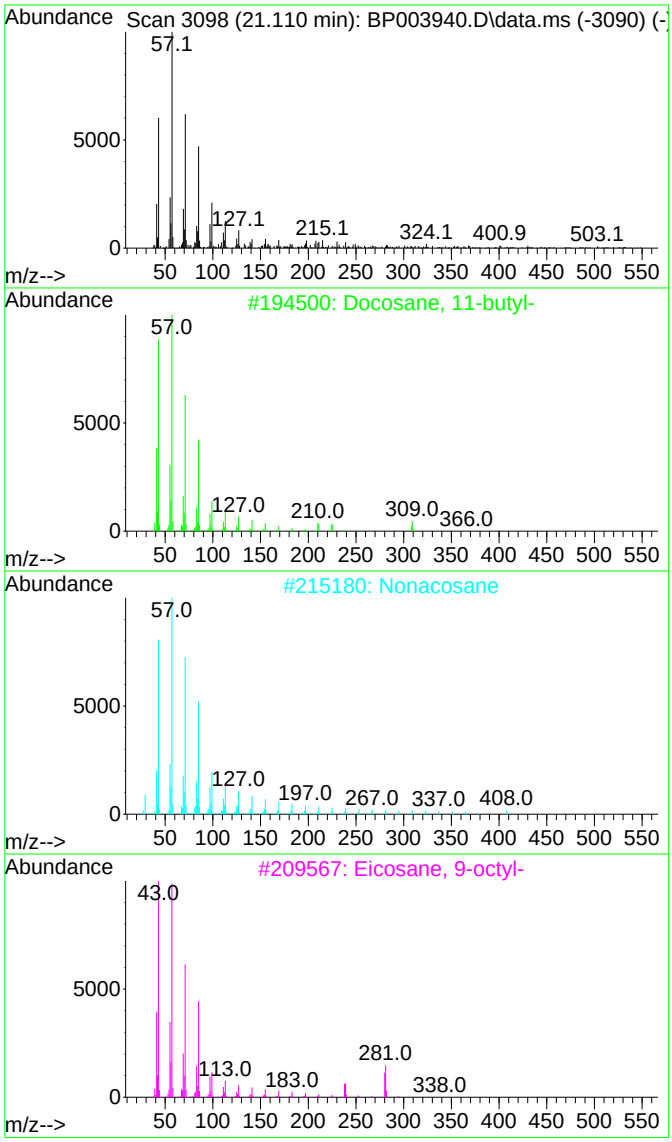
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

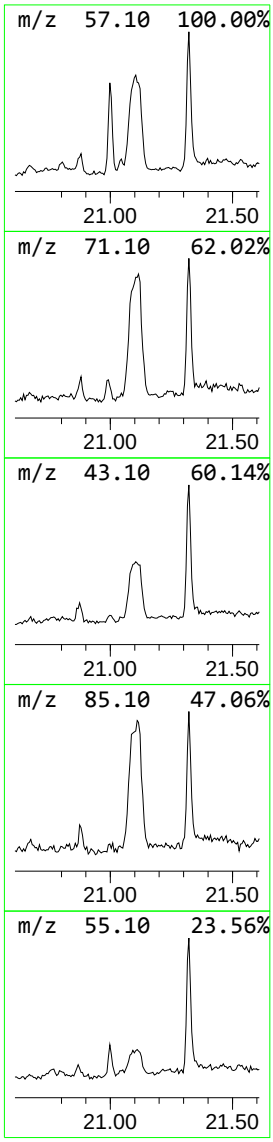
****

Peak Number 7 Docosane, 11-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.110	6.05 ng	453954	Chrysene-d12	21.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	89
2	Nonacosane	408	C29H60	000630-03-5	89
3	Eicosane, 9-octyl-	394	C28H58	013475-77-9	86
4	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	83
5	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111220\
Data File : BP003940.D
Acq On : 12 Nov 2020 15:59
Operator : CG/JU
Sample : L4719-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-3-S

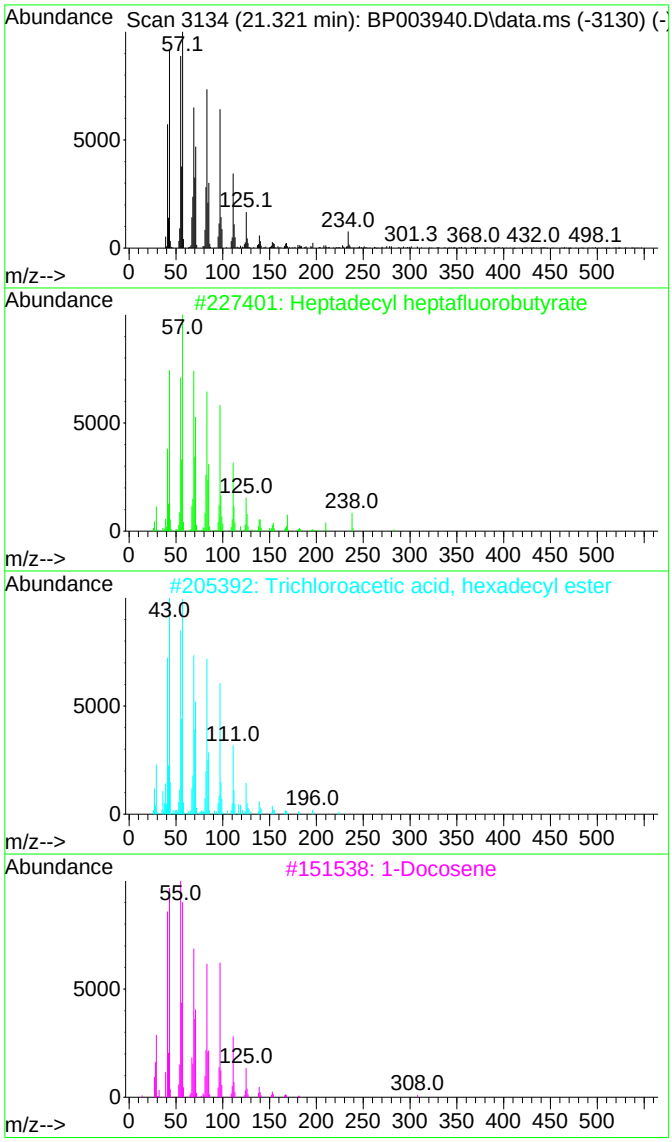
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

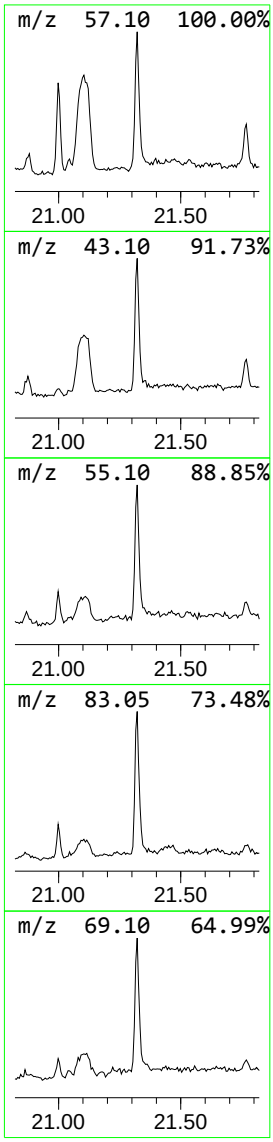
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.321	6.70 ng	501955	Chrysene-d12	21.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	1-Docosene	308	C22H44	001599-67-3	92
4	Cyclooctacosane	392	C28H56	000297-24-5	91
5	Cyclotetracosane	336	C24H48	000297-03-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111220\
Data File : BP003940.D
Acq On : 12 Nov 2020 15:59
Operator : CG/JU
Sample : L4719-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 2,2-di...	2.928	69.6	ng	2982450	1	8.281	856827	20.0
Cyclohexane	3.087	5.8	ng	250276	1	8.281	856827	20.0
Butane, 2-metho...	3.175	10.3	ng	440447	1	8.281	856827	20.0
D-Allose	14.692	2.0	ng	137371	3	14.904	1362600	20.0
Tridecane, 1-iodo-	19.733	7.0	ng	527155	5	21.669	1499440	20.0
Docosane, 11-bu...	21.110	6.0	ng	453954	5	21.669	1499440	20.0
Heptadecyl hept...	21.321	6.7	ng	501955	5	21.669	1499440	20.0