LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102820\
Data File : BP003769.D
Acq On : 28 Oct 2020 14:25
Operator : CG/JU
Sample : L4529-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-T3

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-BP101920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003769.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.087	29	34	53	rVB	1539812	1975611	39.56%	6.143%
2	3.252	56	62	73	rVV2	71194	155890	3.12%	0.485%
3	3.346	73	78	93	rVB	162151	226652	4.54%	0.705%
4	6.011	521	531	541	rBV	1480524	2279330	45.65%	7.087%
5	7.658	802	811	824	rBV	1386840	2313441	46.33%	7.193%
6	8.069	875	881	888	rBV	62729	96215	1.93%	0.299%
7	8.510	949	956	964	rBV	411205	652214	13.06%	2.028%
8	9.675	1146	1154	1162	rBV	904099	1470554	29.45%	4.572%
9	11.352	1432	1439	1452	rBV	501349	841648	16.85%	2.617%
10	13.740	1837	1845	1852	rBV	2098322	3056291	61.20%	9.503%
11	13.993	1882	1888	1901	rVB	261872	407830	8.17%	1.268%
12	14.528	1973	1979	1988	rVB	308447	407345	8.16%	1.267%
13	15.110	2071	2078	2087	rBV	771679	1122030	22.47%	3.489%
14	16.192	2257	2262	2272	rVB2	51288	73143	1.46%	0.227%
15	16.587	2320	2329	2343	rBV	1890554	2753465	55.14%	8.561%
16	17.834	2534	2541	2547	rBV	971964	1357546	27.19%	4.221%
17	18.645	2674	2679	2687	rBV	356267	533797	10.69%	1.660%
18	19.451	2812	2816	2821	rBV2	38203	53506	1.07%	0.166%
19	19.839	2879	2882	2889	rBV3	47820	75833	1.52%	0.236%
20	20.304	2955	2961	2968	rBV	4253453	4993532	100.00%	15.526%
21	21.475	3152	3160	3164	rBV2	395784	587002	11.76%	1.825%
22	21.510	3164	3166	3170	rVV	111651	131897	2.64%	0.410%
23	21.557	3170	3174	3182	rVB	215972	281595	5.64%	0.876%
24	21.851	3218	3224	3229	rBV	1246531	1659015	33.22%	5.158%
25	21.939	3236	3239	3244	rVB4	45558	61507	1.23%	0.191%
26	22.422	3317	3321	3332	rBV4	76864	164756	3.30%	0.512%
27	22.945	3406	3410	3414	rVB2	106523	144705	2.90%	0.450%
28	23.104	3432	3437	3448	rVB	1299435	2007426	40.20%	6.242%
29	23.521	3504	3508	3515	rVB	125654	194184	3.89%	0.604%
30	24.180	3616	3620	3630	rVB2	113612	220827	4.42%	0.687%
31	24.427	3655	3662	3673	rVB2	787154	1679587	33.64%	5.222%
32	24.939	3744	3749	3758	rVB2	90516	183121	3.67%	0.569%

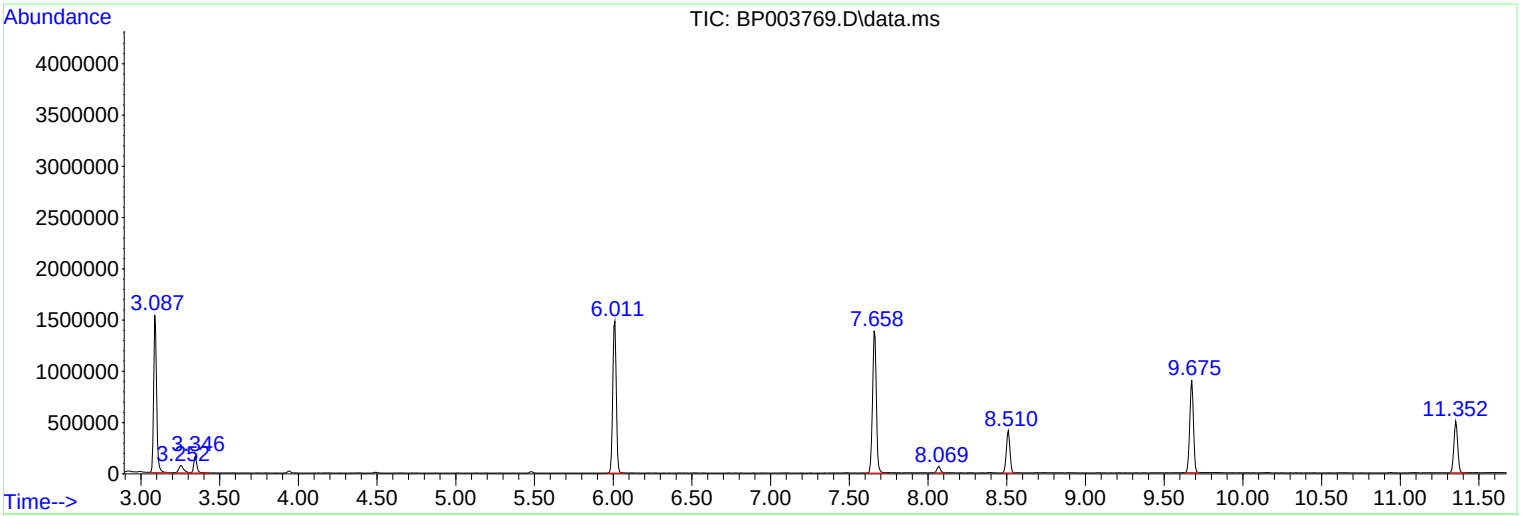
Sum of corrected areas: 32161495

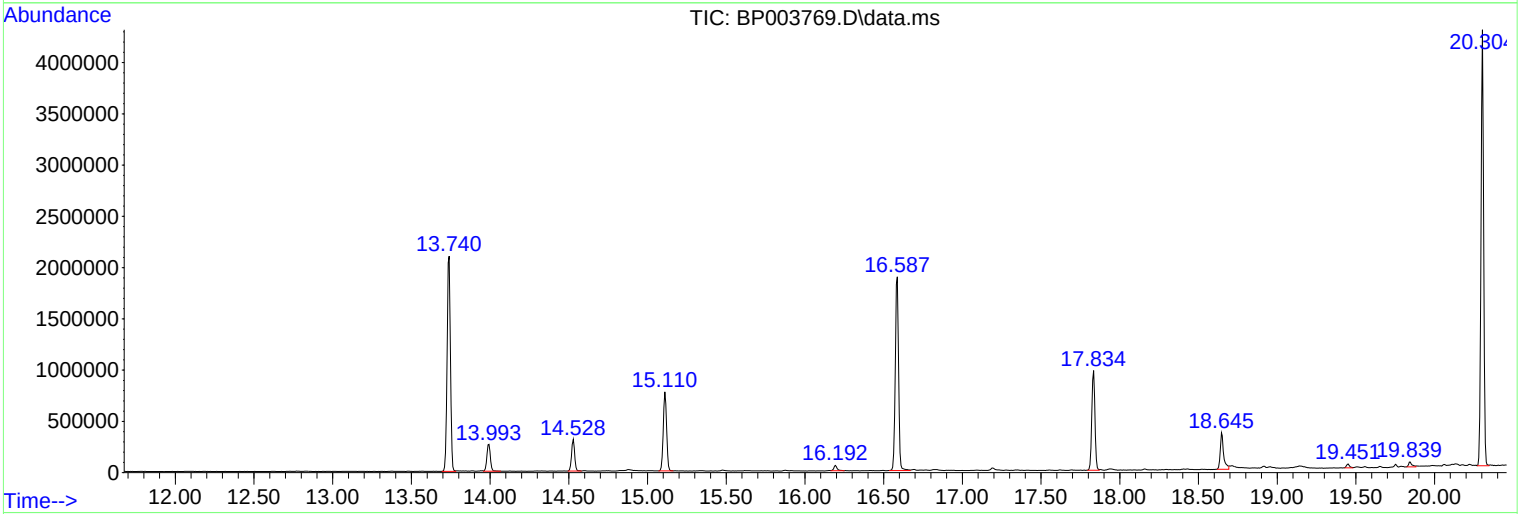
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102820\
Data File : BP003769.D
Acq On : 28 Oct 2020 14:25
Operator : CG/JU
Sample : L4529-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

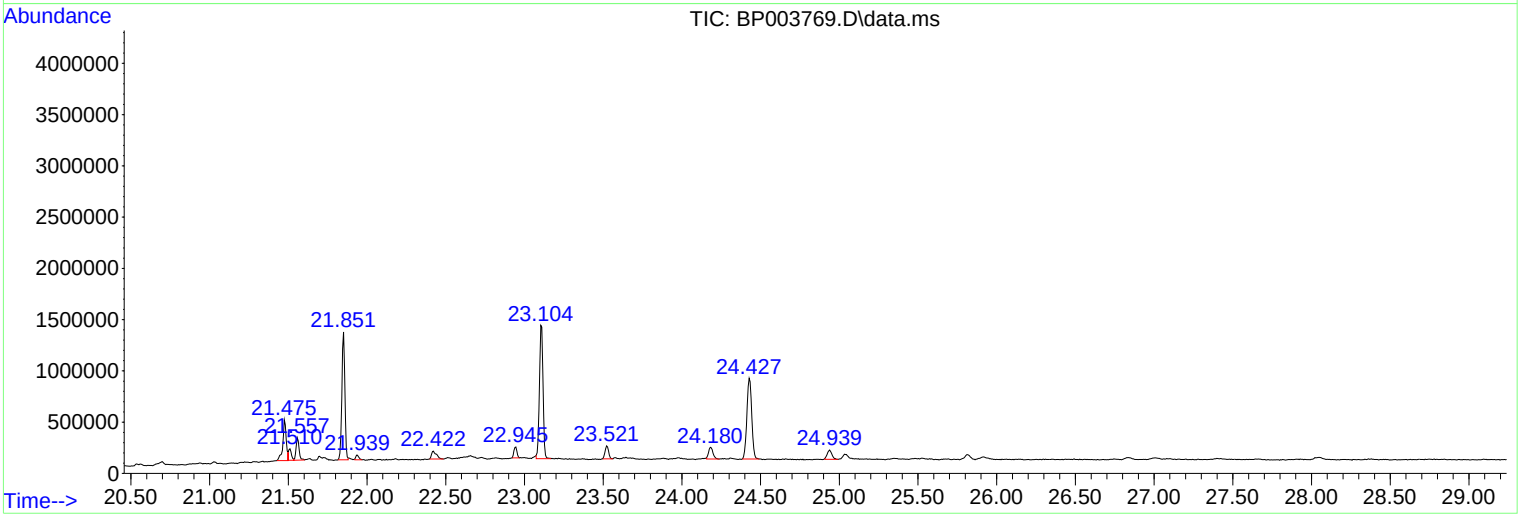
Instrument :
BNA_P
ClientSampleId :
TP-T3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.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\BP102820\
Data File : BP003769.D
Acq On : 28 Oct 2020 14:25
Operator : CG/JU
Sample : L4529-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-T3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

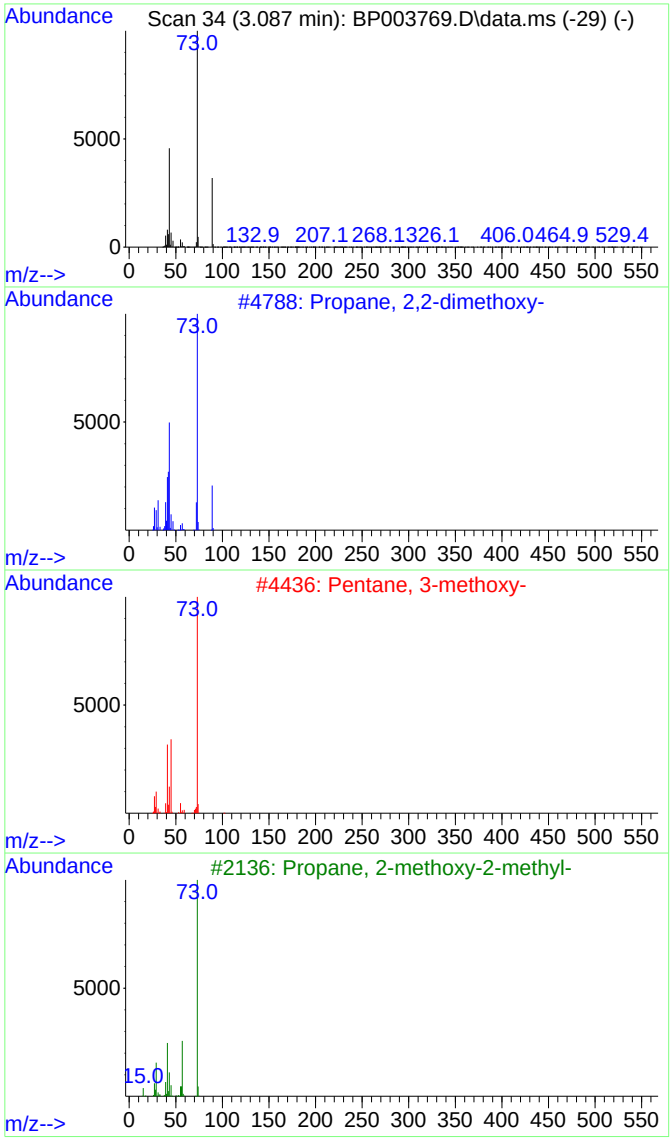
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

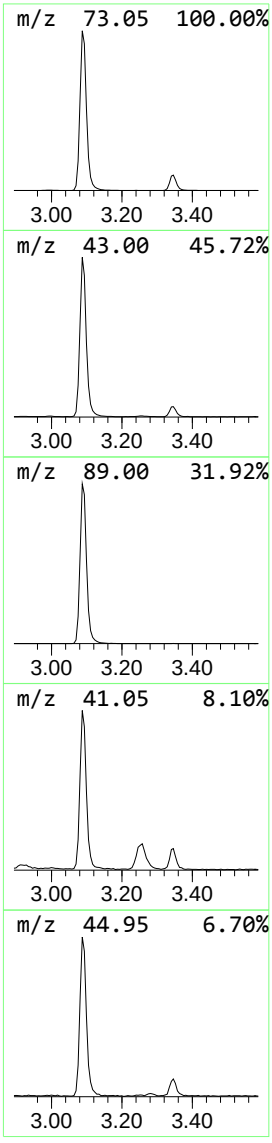
****

Peak Number 1 unknown3.08 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	60.58 ng	1975610	1,4-Dichlorobenzene-d4	8.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102820\
Data File : BP003769.D
Acq On : 28 Oct 2020 14:25
Operator : CG/JU
Sample : L4529-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-T3

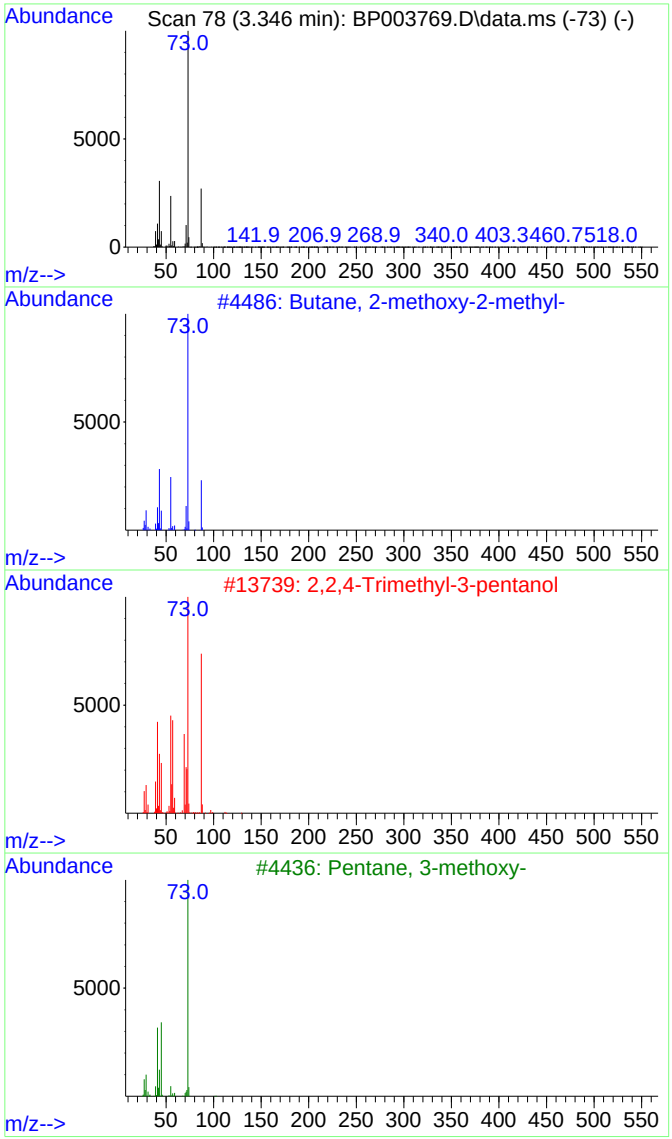
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

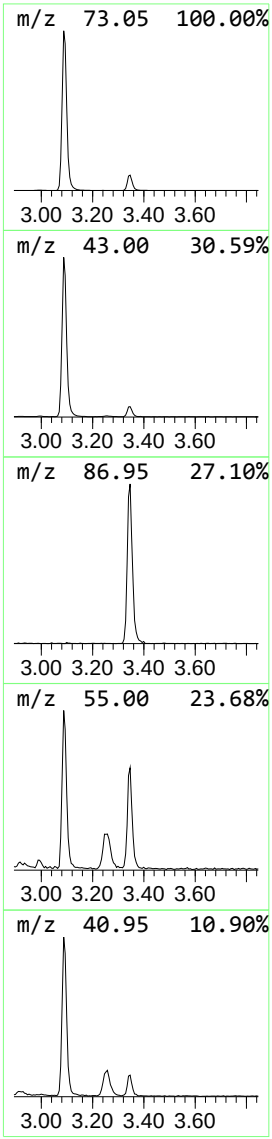
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.346	6.95 ng	226652	1,4-Dichlorobenzene-d4	8.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102820\
Data File : BP003769.D
Acq On : 28 Oct 2020 14:25
Operator : CG/JU
Sample : L4529-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-T3

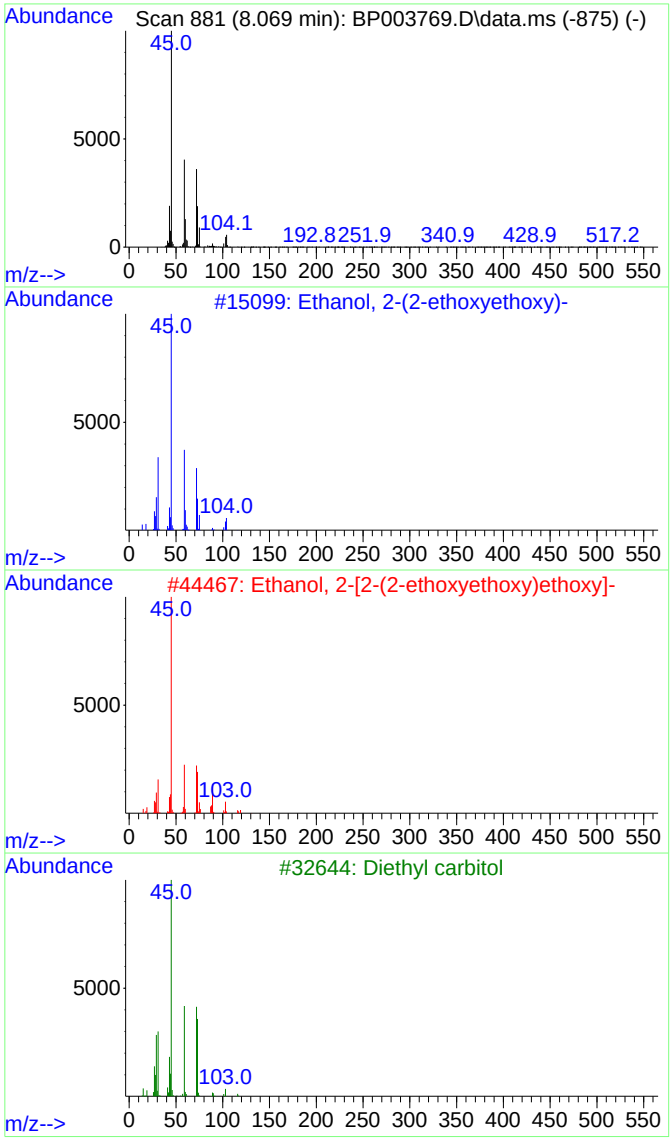
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

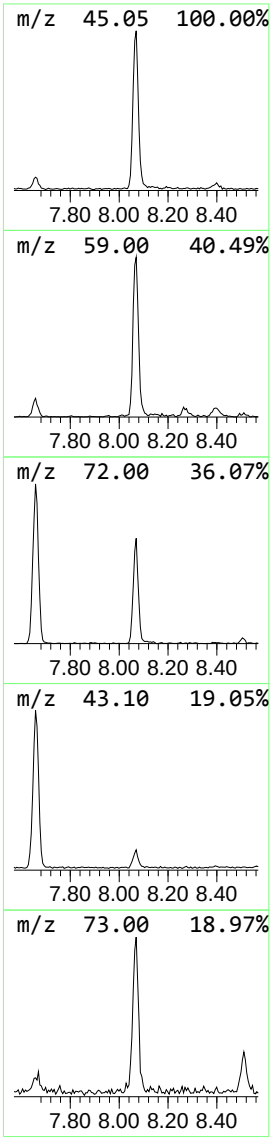
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	2.95 ng	96215	1,4-Dichlorobenzene-d4	8.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	50
3	Diethyl carbitol	162	C8H18O3	000112-36-7	45
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5	Trimethylene glycol monomethyl e...	90	C4H10O2	001589-49-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102820\
Data File : BP003769.D
Acq On : 28 Oct 2020 14:25
Operator : CG/JU
Sample : L4529-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-T3

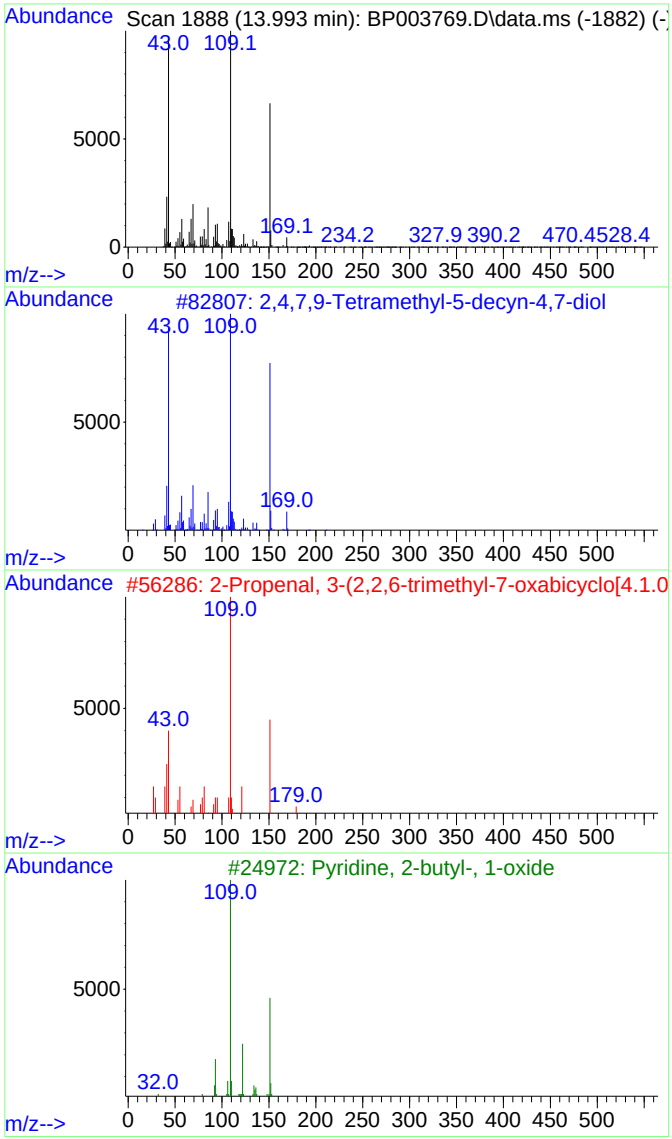
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

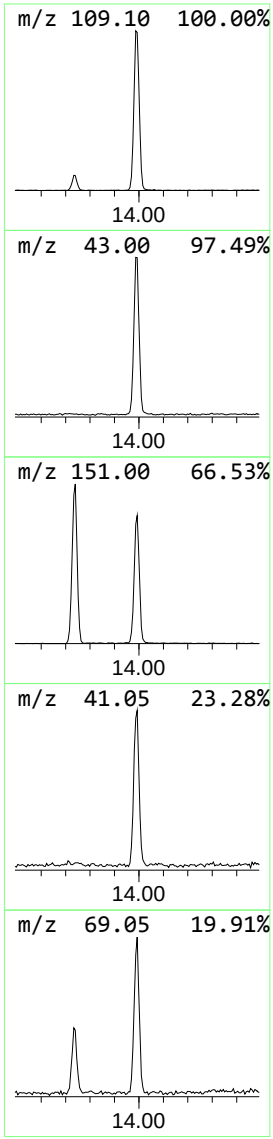
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.993	7.27 ng	407830	Acenaphthene-d10	15.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	64
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
4	Metacetamol	151	C8H9NO2	000621-42-1	53
5	1,2-Diazaspiro[4.4]nonen-3-carbo...	252	C14H24N2O2	1000164-25-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102820\
Data File : BP003769.D
Acq On : 28 Oct 2020 14:25
Operator : CG/JU
Sample : L4529-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-T3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

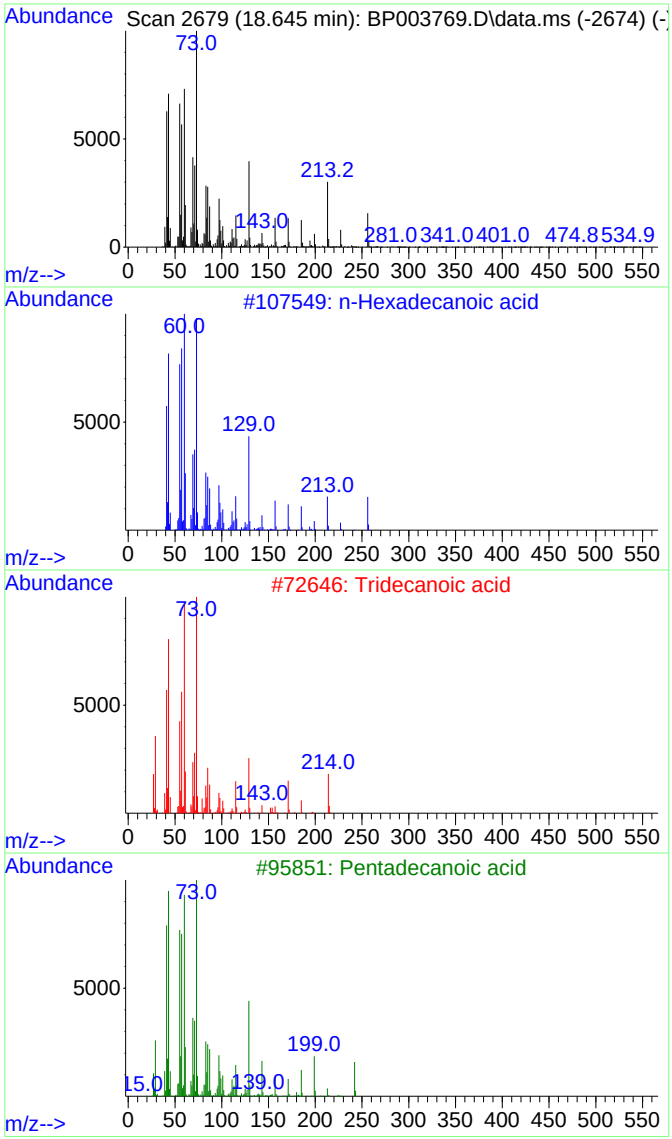
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

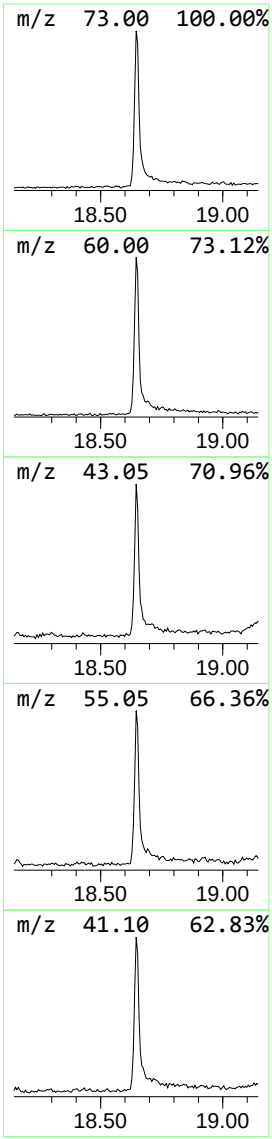
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.645	7.86 ng	533797	Phenanthrene-d10	17.834

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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102820\
Data File : BP003769.D
Acq On : 28 Oct 2020 14:25
Operator : CG/JU
Sample : L4529-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-T3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

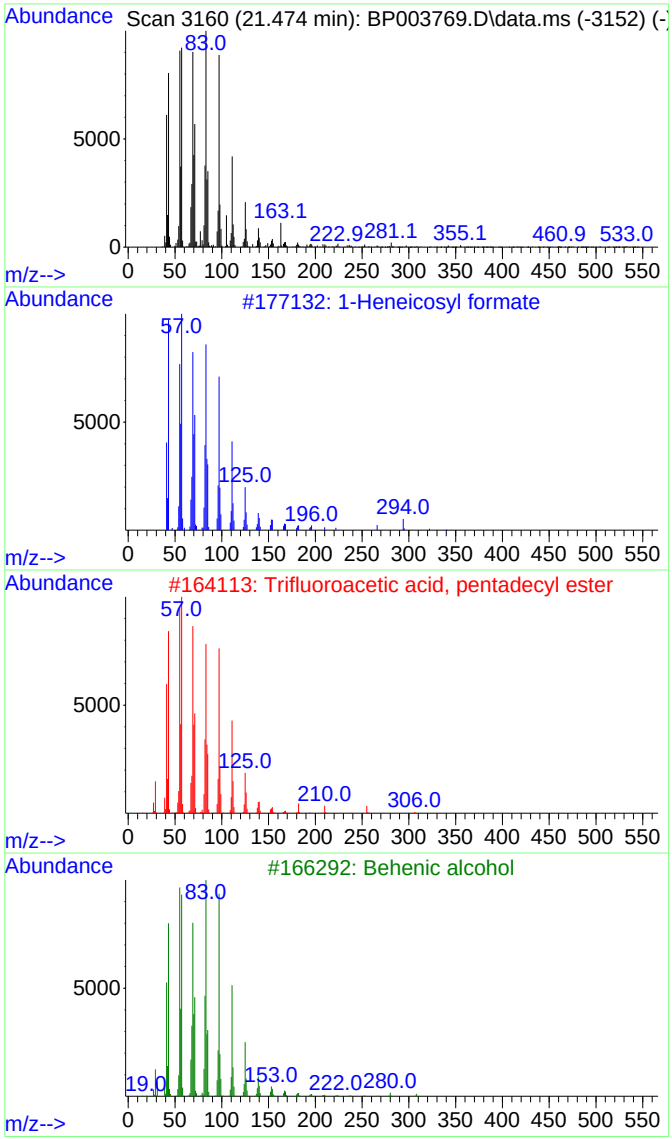
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

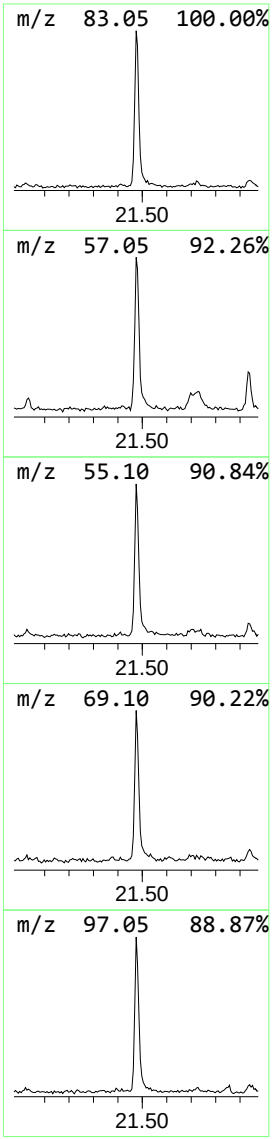
****

Peak Number 7 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.474	7.08 ng	587002	Chrysene-d12	21.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102820\
Data File : BP003769.D
Acq On : 28 Oct 2020 14:25
Operator : CG/JU
Sample : L4529-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-T3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

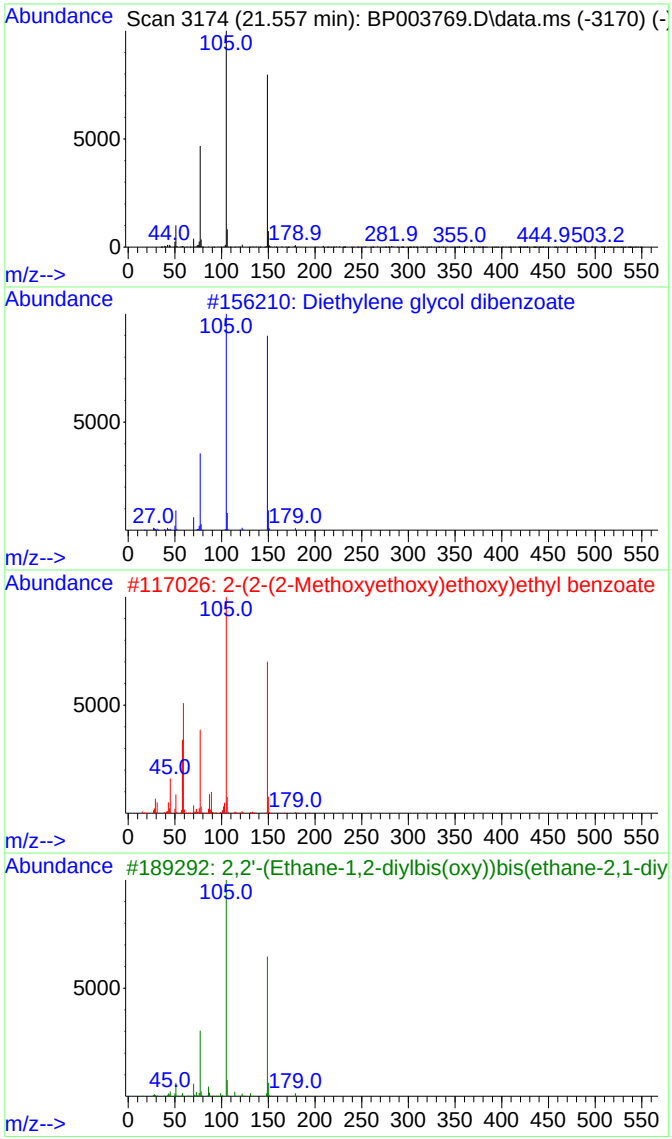
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

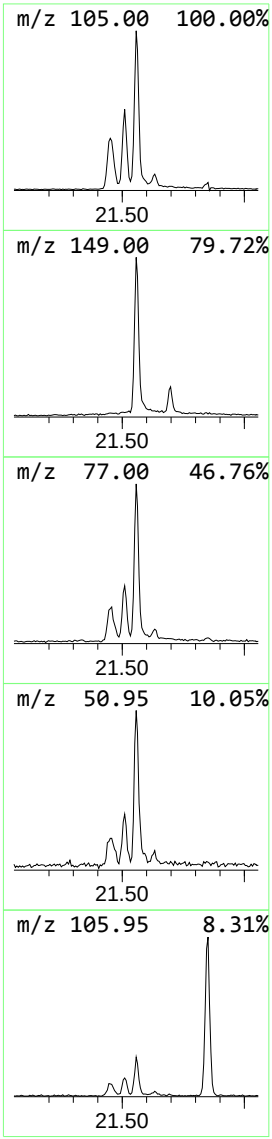
****

Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.557	3.39 ng	281595	Chrysene-d12	21.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
2	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	74
4	Ethanol, 2-(4-phenoxyphenoxy)-, ...	334	C21H18O4	055191-59-8	72
5	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102820\
Data File : BP003769.D
Acq On : 28 Oct 2020 14:25
Operator : CG/JU
Sample : L4529-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-T3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

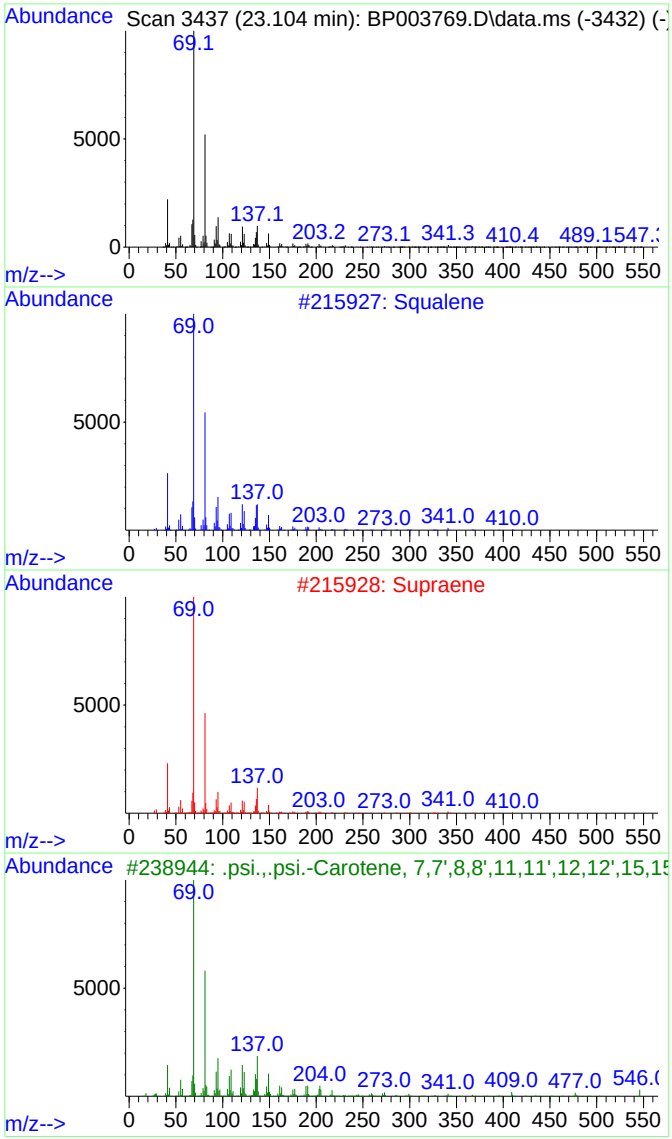
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

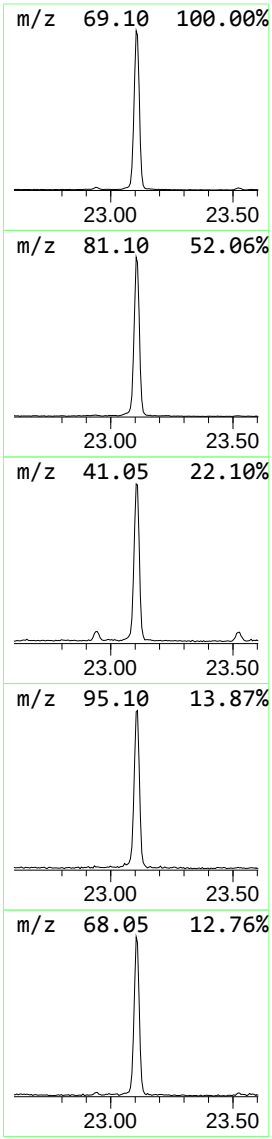
****

Peak Number 9 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.104	24.20 ng	2007430	Chrysene-d12	21.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	95
2	Supraene	410	C30H50	007683-64-9	91
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102820\
Data File : BP003769.D
Acq On : 28 Oct 2020 14:25
Operator : CG/JU
Sample : L4529-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-T3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

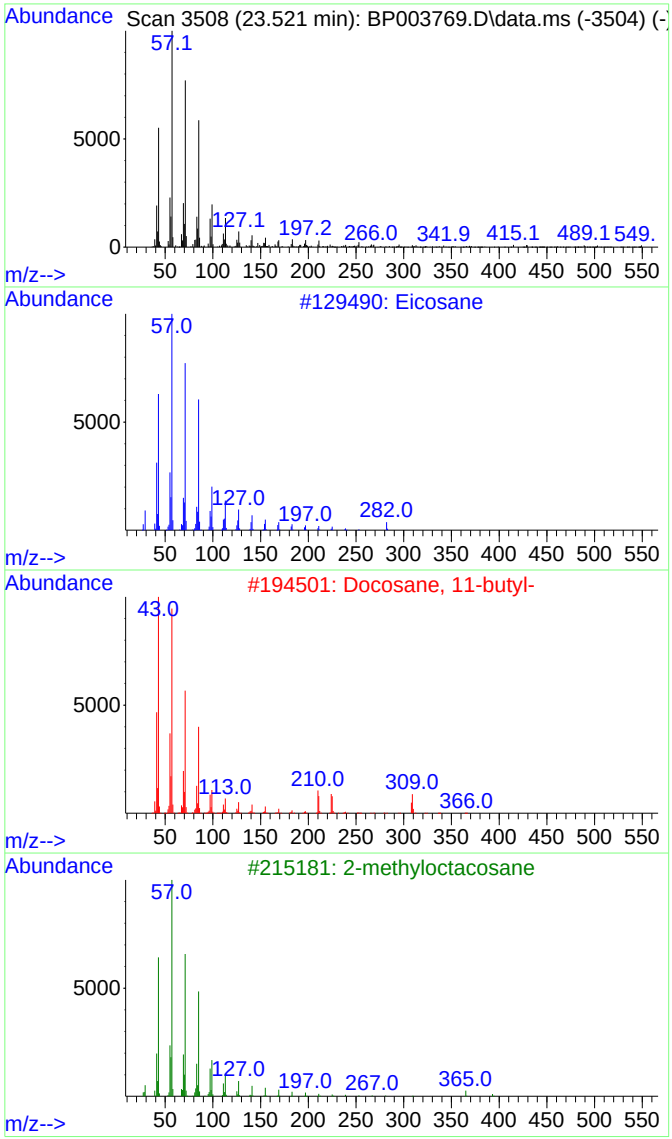
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

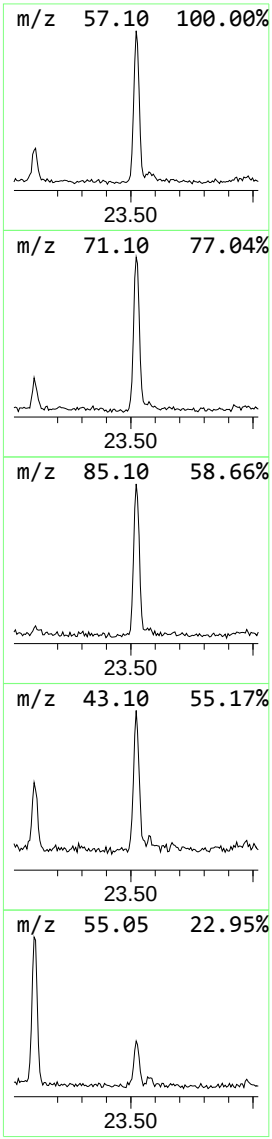
****

Peak Number 10 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.522	2.31 ng	194184	Perylene-d12	24.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptacosane	380	C27H56	000593-49-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102820\
Data File : BP003769.D
Acq On : 28 Oct 2020 14:25
Operator : CG/JU
Sample : L4529-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-T3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

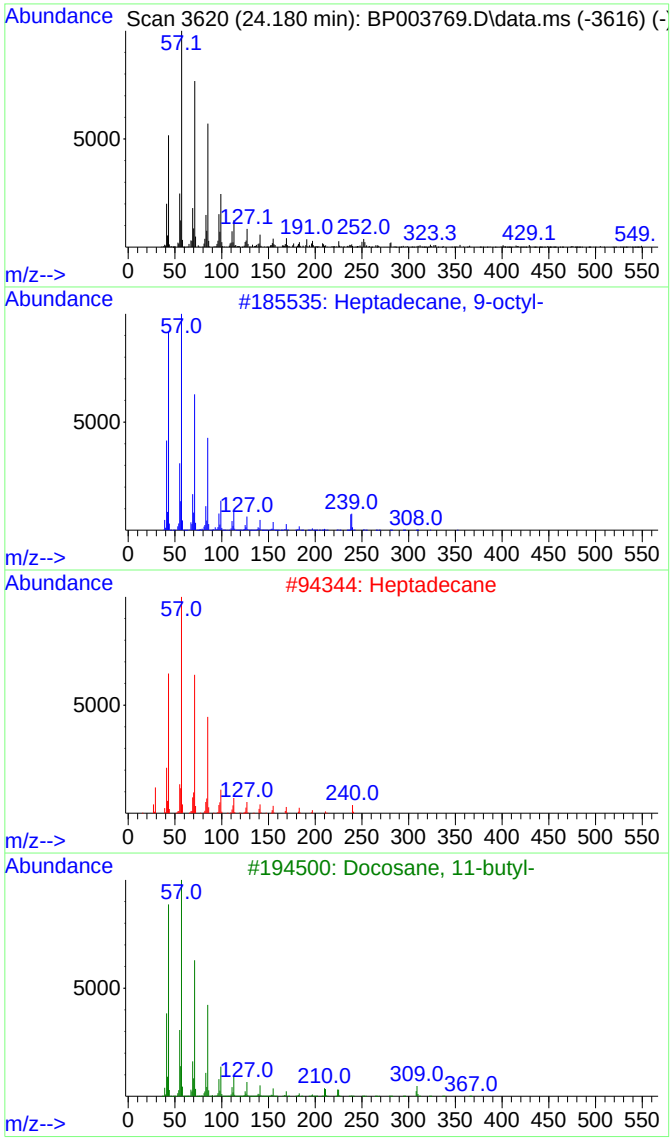
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

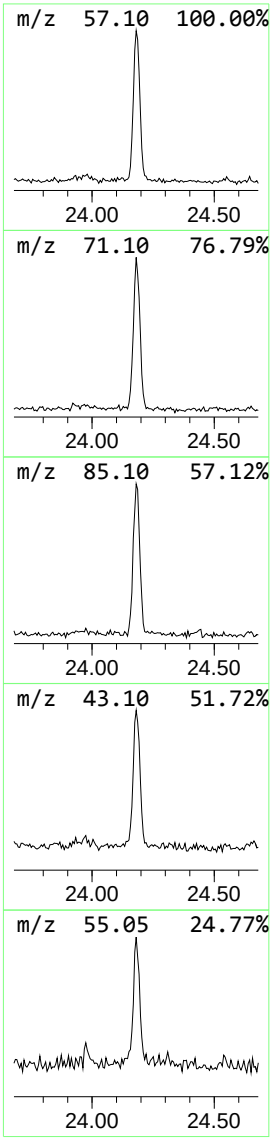
****

Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.180	2.63 ng	220827	Perylene-d12	24.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2	Heptadecane	240	C17H36	000629-78-7	91
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	89
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heneicosane	296	C21H44	000629-94-7	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102820\
Data File : BP003769.D
Acq On : 28 Oct 2020 14:25
Operator : CG/JU
Sample : L4529-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-T3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

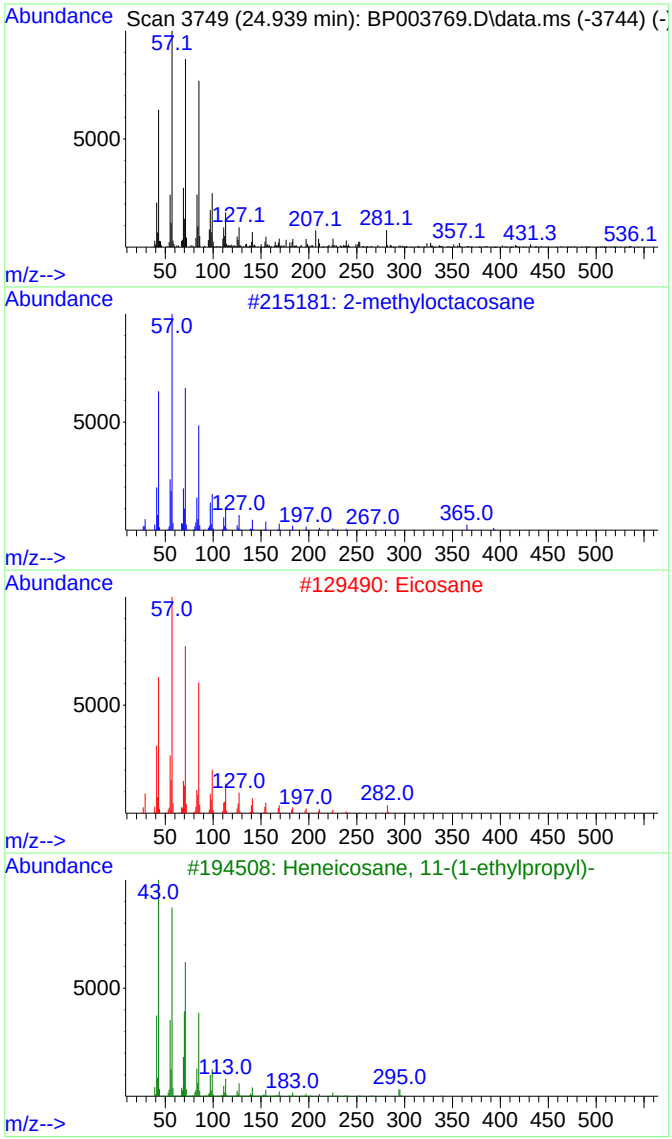
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

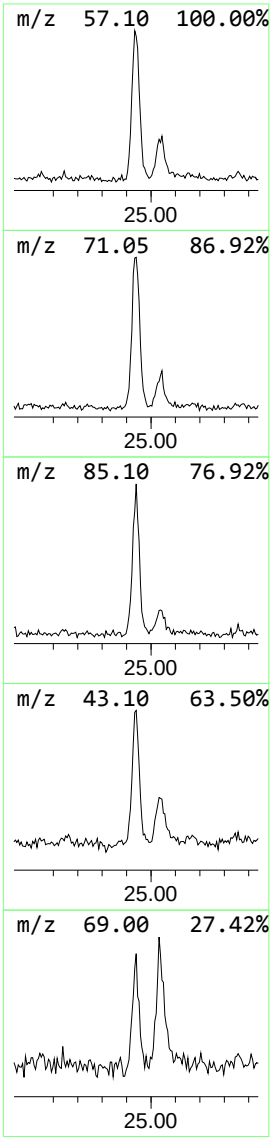
****

Peak Number 12 2-methyloctacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.939	2.18 ng	183121	Perylene-d12	24.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	90
2	Eicosane	282	C20H42	000112-95-8	87
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
4	Heneicosane	296	C21H44	000629-94-7	86
5	Heptadecane	240	C17H36	000629-78-7	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102820\
Data File : BP003769.D
Acq On : 28 Oct 2020 14:25
Operator : CG/JU
Sample : L4529-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-T3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.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
unknown3.08	3.087	60.6	ng	1975610	1	8.510	652214	20.0
Butane, 2-metho...	3.346	7.0	ng	226652	1	8.510	652214	20.0
Ethanol, 2-(2-e...	8.069	3.0	ng	96215	1	8.510	652214	20.0
2,4,7,9-Tetrame...	13.993	7.3	ng	407830	3	15.110	1122030	20.0
n-Hexadecanoic ...	18.645	7.9	ng	533797	4	17.834	1357550	20.0
1-Heneicosyl fo...	21.474	7.1	ng	587002	5	21.851	1659020	20.0
Diethylene glyc...	21.557	3.4	ng	281595	5	21.851	1659020	20.0
Squalene	23.104	24.2	ng	2007430	5	21.851	1659020	20.0
Eicosane	23.522	2.3	ng	194184	6	24.427	1679590	20.0
Heptadecane, 9-...	24.180	2.6	ng	220827	6	24.427	1679590	20.0
2-methyloctacosane	24.939	2.2	ng	183121	6	24.427	1679590	20.0