LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126250.D
Acq On : 18 Dec 2021 13:02
Operator : JU/CG
Sample : M5082-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(35-52)

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-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126250.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	14	rVB	747857	910126	17.02%	2.095%
2	2.234	19	25	31	rBV	87775	116231	2.17%	0.268%
3	3.287	202	204	210	rBV	33103	61878	1.16%	0.142%
4	5.034	492	501	509	rBV	1109510	1420533	26.57%	3.270%
5	5.434	563	569	572	rBV	4681099	5103920	95.46%	11.750%
6	5.828	633	636	640	rVB	164630	149869	2.80%	0.345%
7	6.445	734	741	744	rBV	4310166	5346614	100.00%	12.309%
8	6.816	800	804	807	rBV	1637139	1329627	24.87%	3.061%
9	7.375	893	899	903	rBV	3073640	3576551	66.89%	8.234%
10	8.004	1002	1006	1017	rBV	69631	112389	2.10%	0.259%
11	8.098	1017	1022	1025	rBV	2155958	1876584	35.10%	4.320%
12	9.175	1200	1205	1209	rBV	4626224	5060203	94.64%	11.649%
13	9.263	1216	1220	1226	rVB2	91763	89859	1.68%	0.207%
14	9.686	1286	1292	1295	rBV5	30630	66670	1.25%	0.153%
15	9.851	1313	1320	1324	rBV	2128057	2003119	37.47%	4.611%
16	10.269	1387	1391	1393	rBV2	88882	90512	1.69%	0.208%
17	10.639	1448	1454	1458	rBV	3139954	3241510	60.63%	7.462%
18	11.304	1562	1567	1569	rBV2	133917	140666	2.63%	0.324%
19	11.339	1569	1573	1576	rVV	2105511	1952627	36.52%	4.495%
20	11.404	1578	1584	1587	rBV3	84053	109108	2.04%	0.251%
21	11.504	1596	1601	1608	rBV2	45938	62037	1.16%	0.143%
22	11.739	1637	1641	1644	rVB	274306	231823	4.34%	0.534%
23	11.869	1659	1663	1666	rVV	284926	257145	4.81%	0.592%
24	11.904	1666	1669	1672	rVB	75772	78108	1.46%	0.180%
25	12.133	1704	1708	1713	rBV3	60538	94199	1.76%	0.217%
26	12.651	1793	1796	1800	rBV2	50061	59592	1.11%	0.137%
27	12.927	1838	1843	1846	rBV	4463673	4712520	88.14%	10.849%
28	13.404	1916	1924	1929	rBV	97543	112941	2.11%	0.260%
29	13.851	1993	2000	2016	rBV	485252	1196774	22.38%	2.755%
30	13.974	2016	2021	2024	rBV	1715295	1695410	31.71%	3.903%
31	14.504	2107	2111	2119	rBV6	35398	80462	1.50%	0.185%
32	14.833	2163	2167	2171	rBV	473684	450887	8.43%	1.038%
33	15.421	2261	2267	2272	rBV	1124425	1426531	26.68%	3.284%
34	16.009	2360	2367	2382	rBV7	59176	221166	4.14%	0.509%

Sum of corrected areas: 43438191

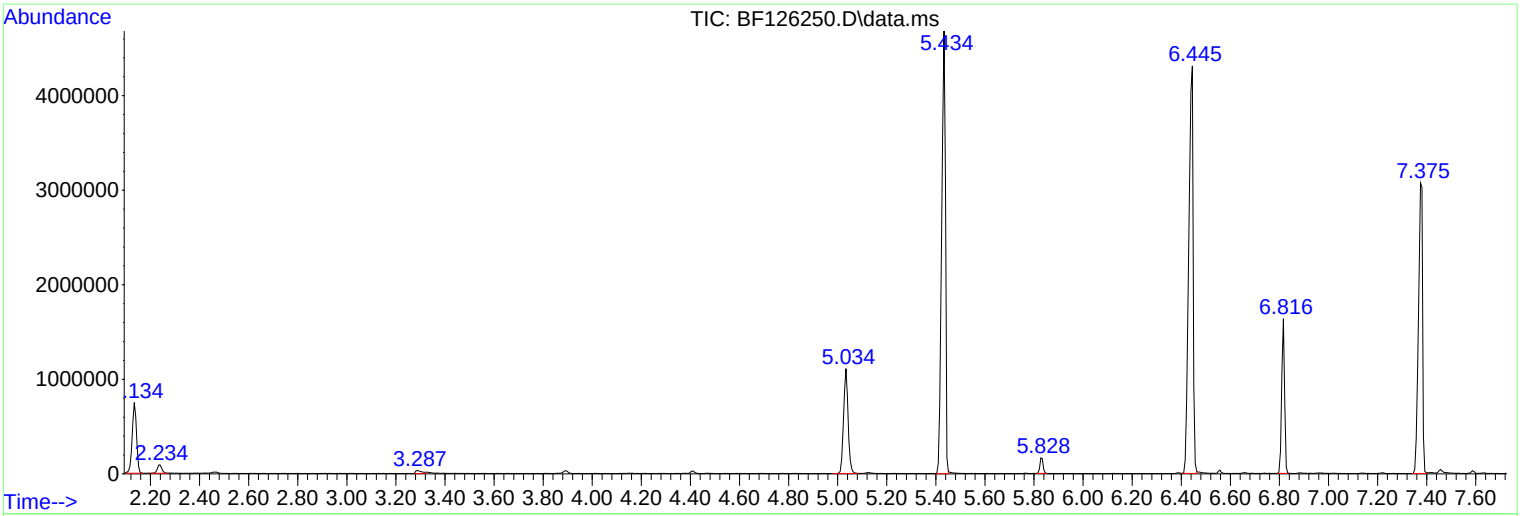
Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(35-52)

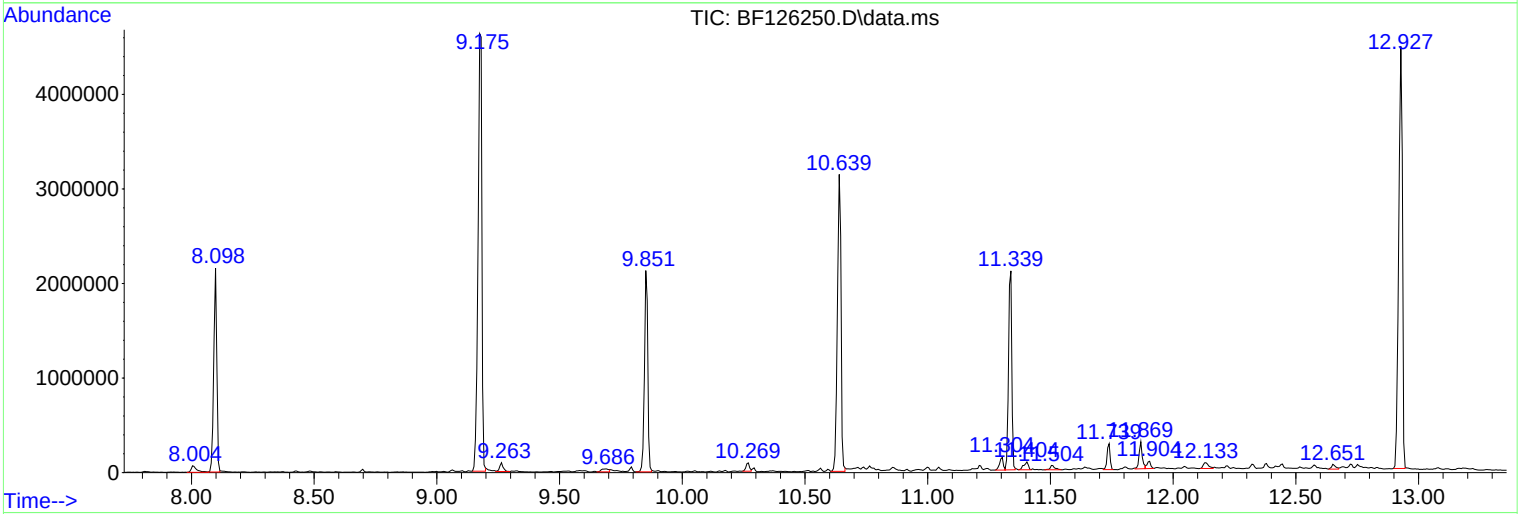
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126250.D
Acq On : 18 Dec 2021 13:02
Operator : JU/CG
Sample : M5082-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

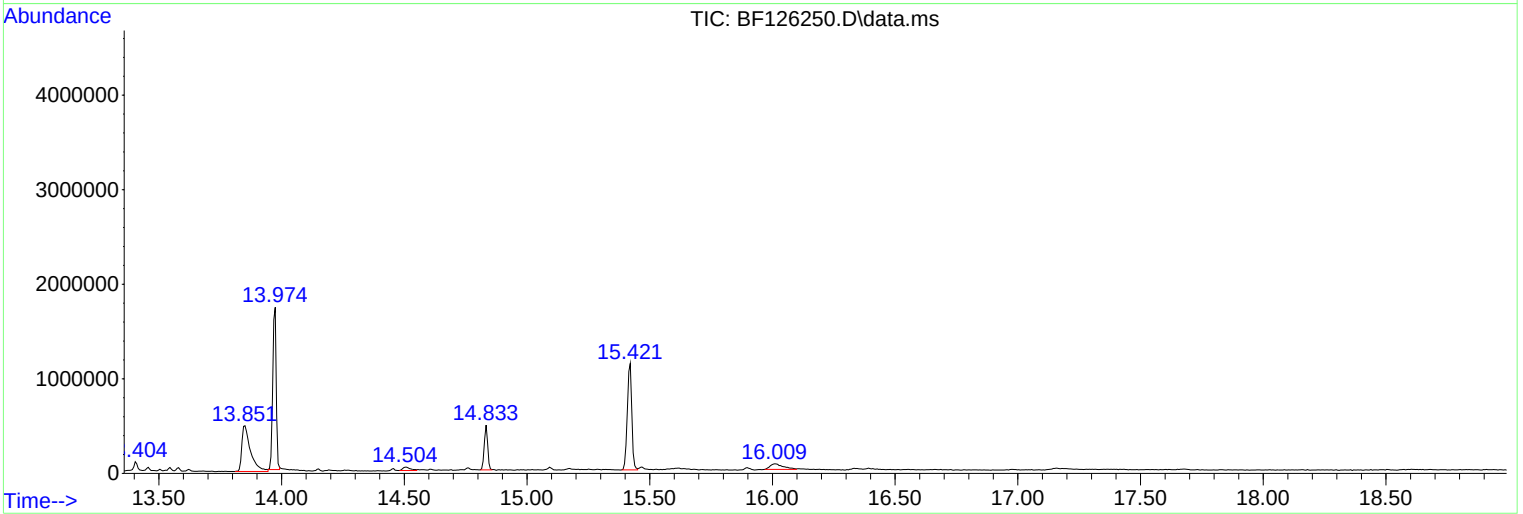
Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(35-52)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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\BF121821\
Data File : BF126250.D
Acq On : 18 Dec 2021 13:02
Operator : JU/CG
Sample : M5082-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(35-52)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

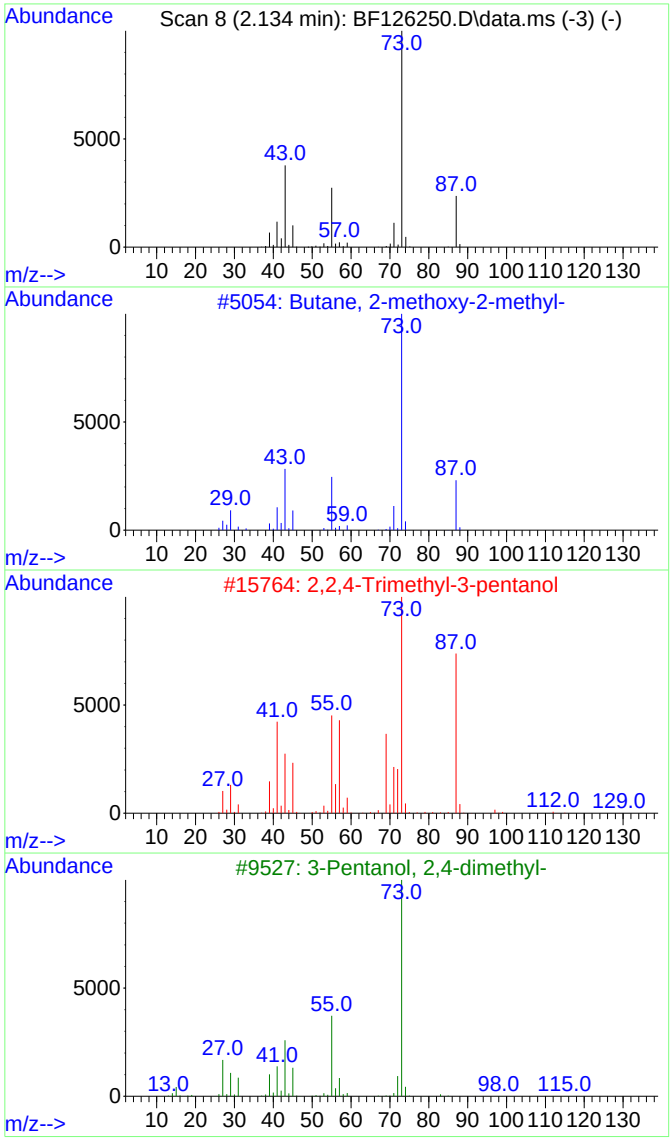
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

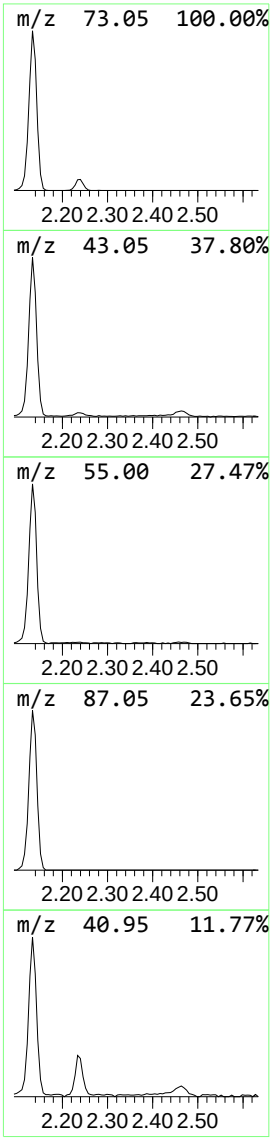
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	13.69 ng	910126	1,4-Dichlorobenzene-d4	6.816

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	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126250.D
Acq On : 18 Dec 2021 13:02
Operator : JU/CG
Sample : M5082-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(35-52)

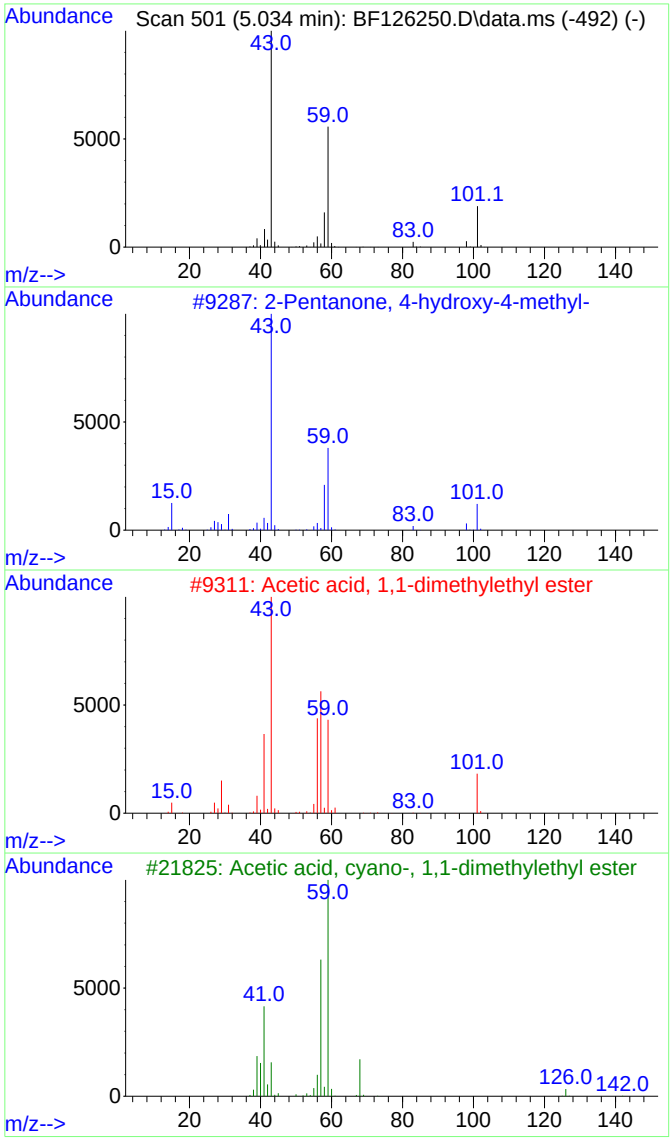
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

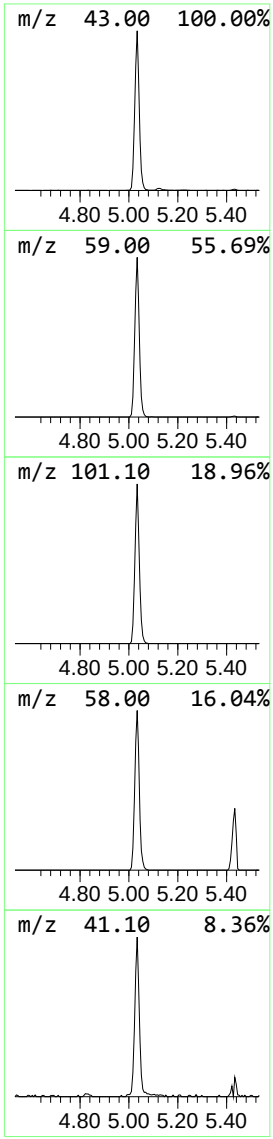
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	21.37 ng	1420530	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126250.D
Acq On : 18 Dec 2021 13:02
Operator : JU/CG
Sample : M5082-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(35-52)

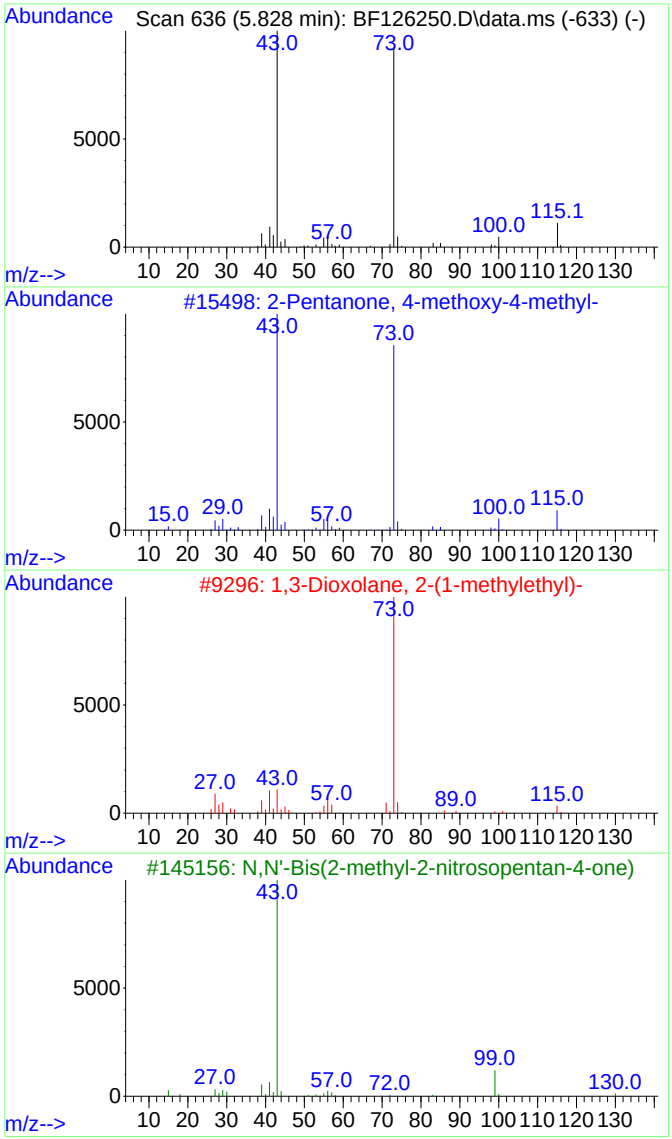
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

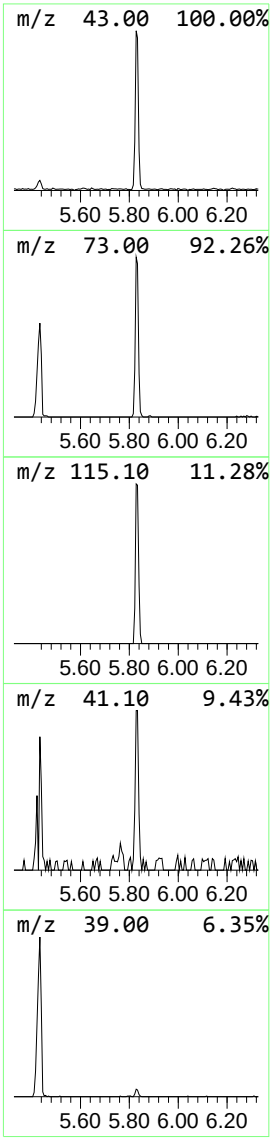
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.828	2.25 ng	149869	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
3	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10
4	N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126250.D
Acq On : 18 Dec 2021 13:02
Operator : JU/CG
Sample : M5082-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(35-52)

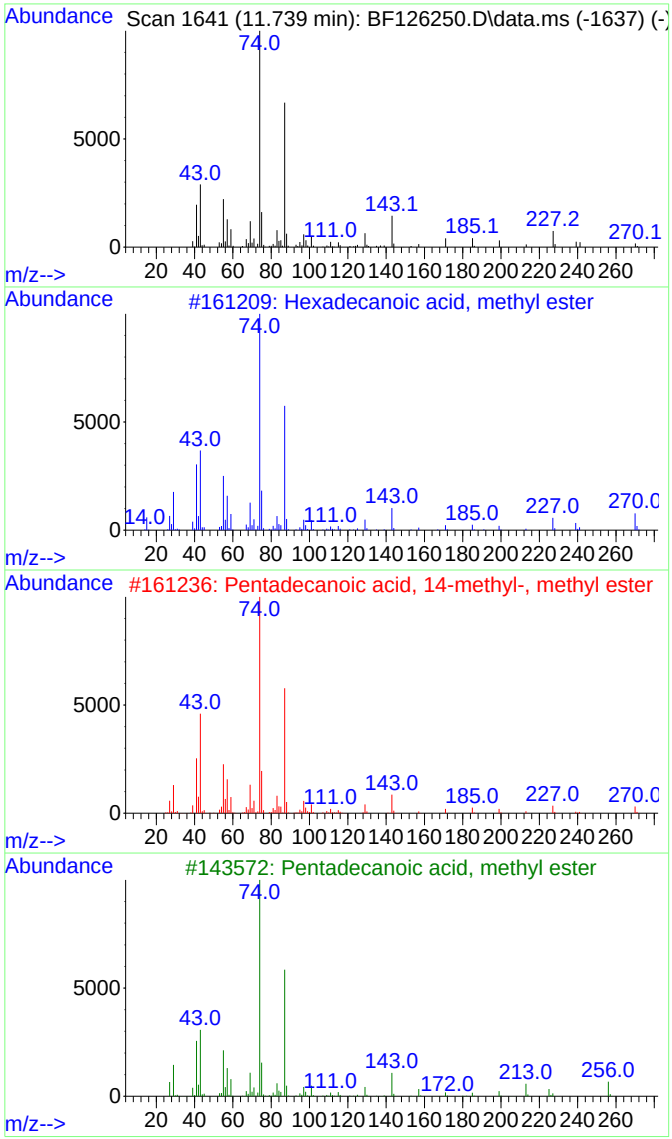
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

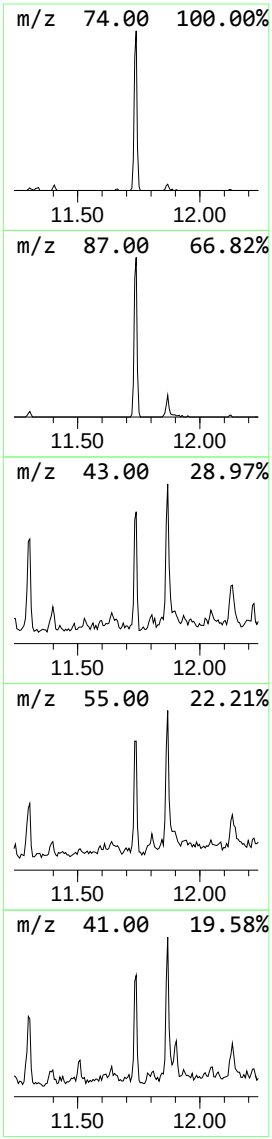
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.739	2.37 ng	231823	Phenanthrene-d10	11.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4	Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	90
5	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126250.D
Acq On : 18 Dec 2021 13:02
Operator : JU/CG
Sample : M5082-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(35-52)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

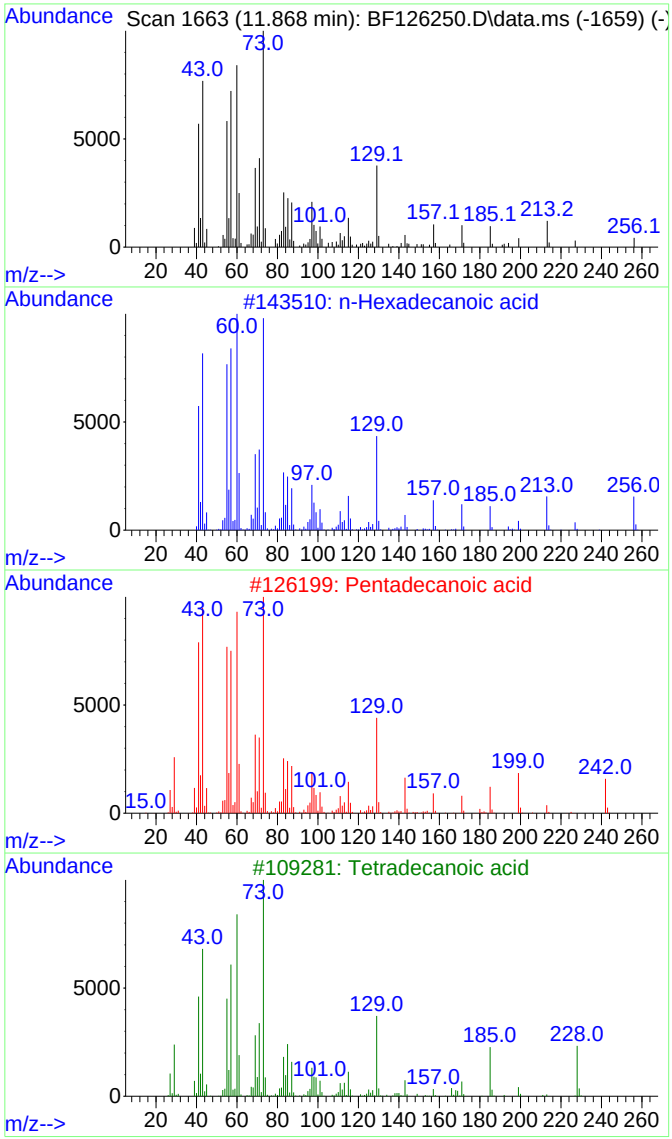
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

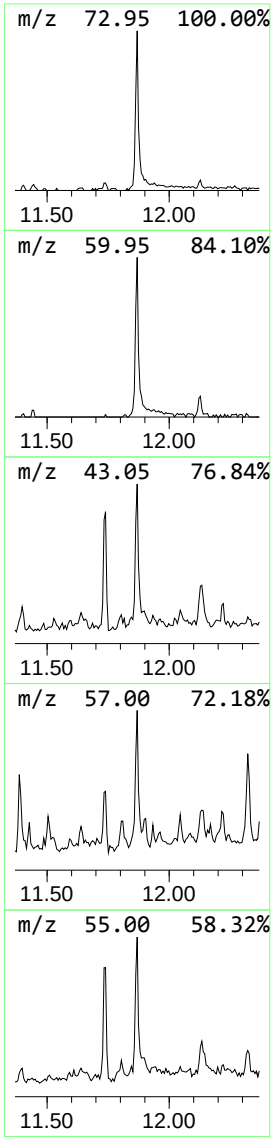
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.868	2.63 ng	257145	Phenanthrene-d10	11.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126250.D
Acq On : 18 Dec 2021 13:02
Operator : JU/CG
Sample : M5082-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(35-52)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

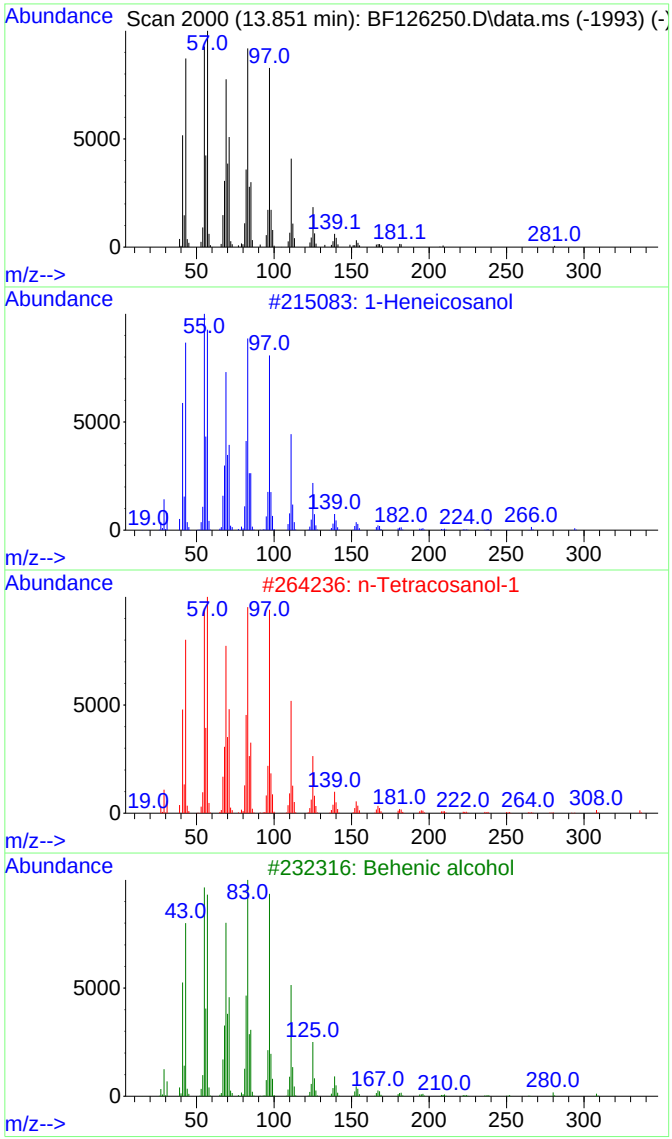
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

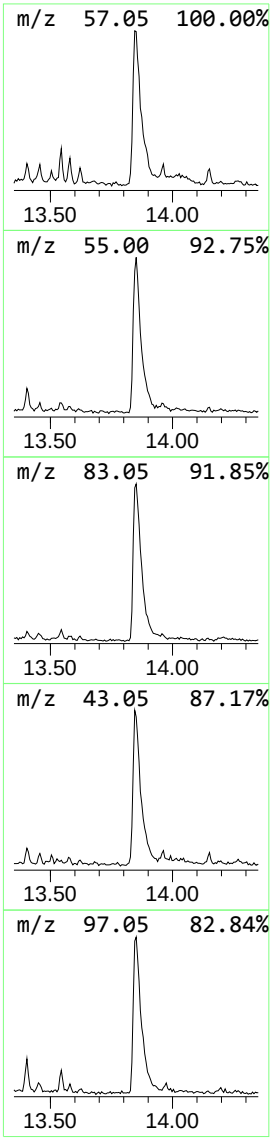
****

Peak Number 6 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	14.12 ng	1196770	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126250.D
Acq On : 18 Dec 2021 13:02
Operator : JU/CG
Sample : M5082-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(35-52)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

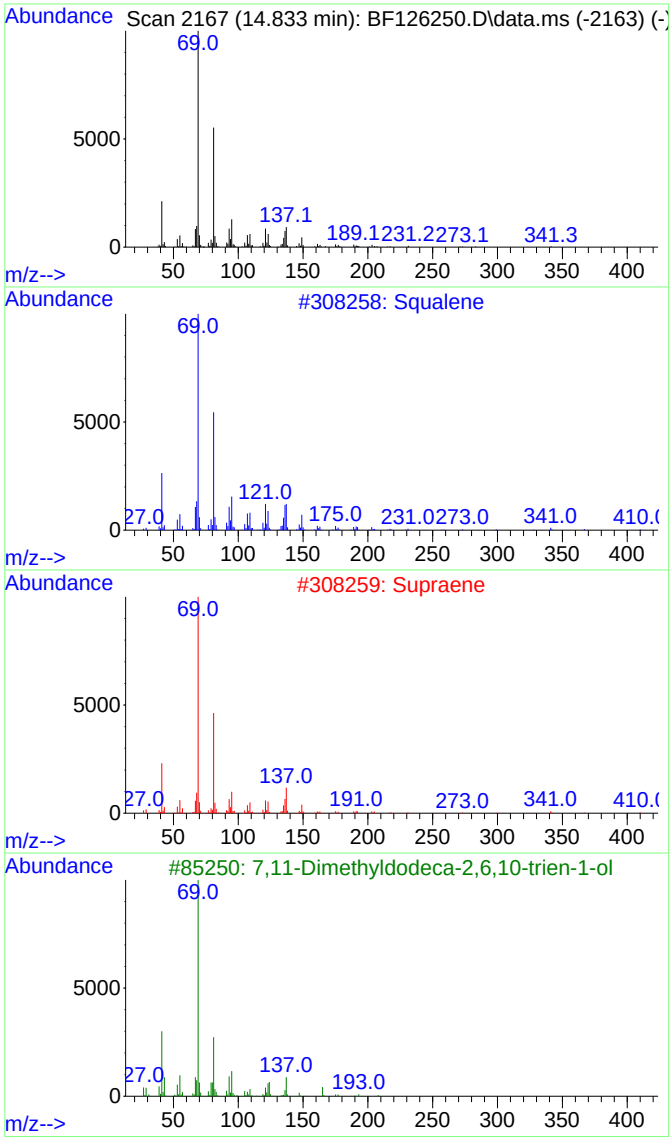
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

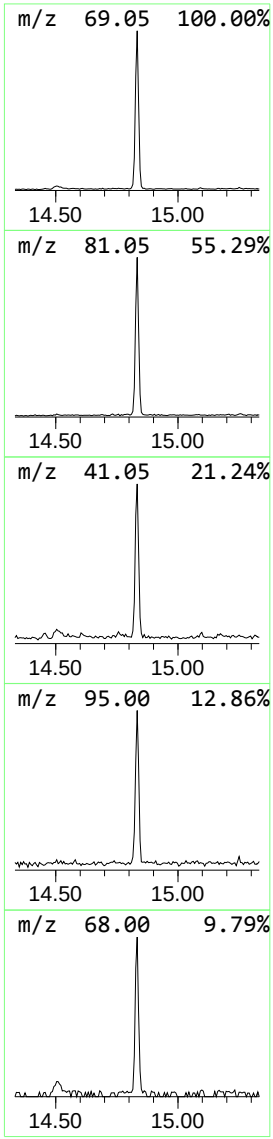
****

Peak Number 7 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	6.32 ng	450887	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	87
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126250.D
Acq On : 18 Dec 2021 13:02
Operator : JU/CG
Sample : M5082-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(35-52)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

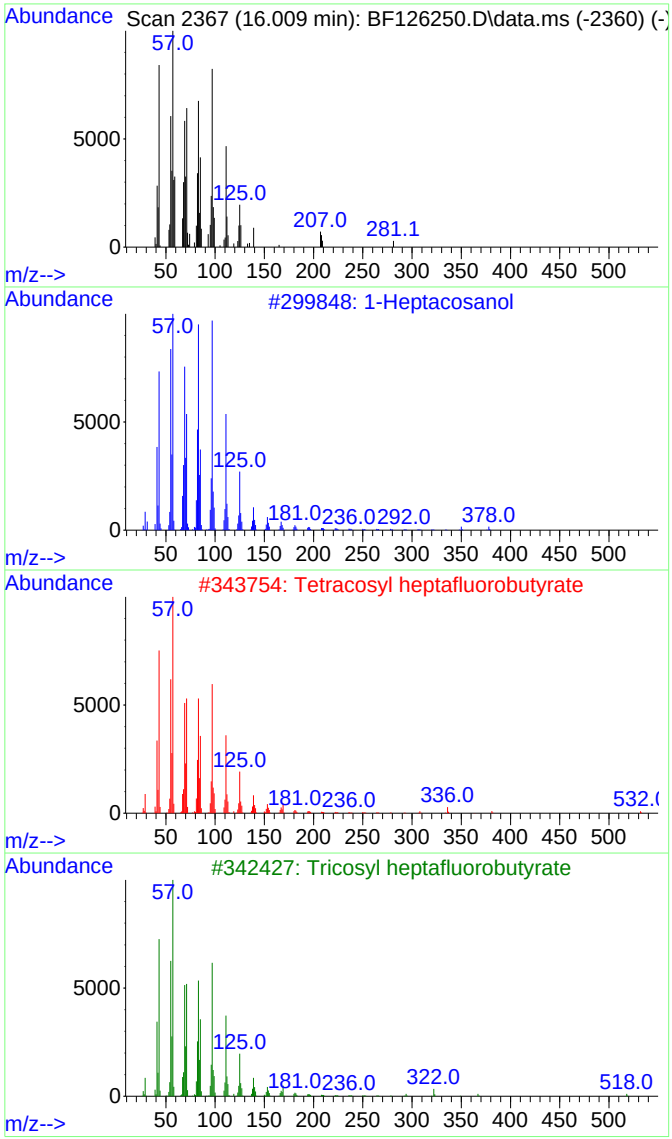
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

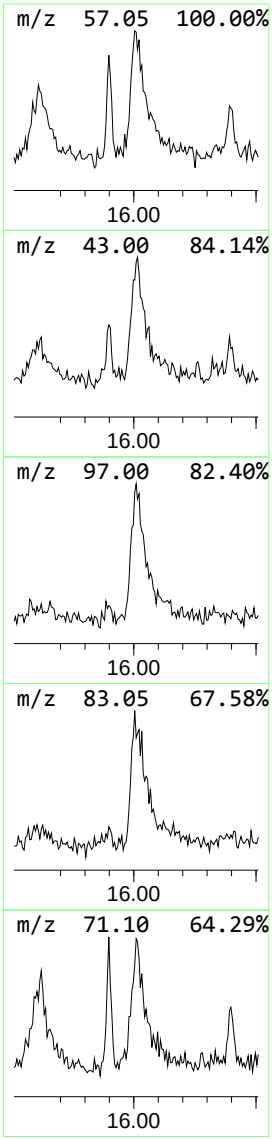
****

Peak Number 8 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.009	3.10 ng	221166	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	90
2	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	87
3	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	87
4	1-Dotriacontanol, acetate	509	C34H68O2	023811-94-1	87
5	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126250.D
Acq On : 18 Dec 2021 13:02
Operator : JU/CG
Sample : M5082-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(35-52)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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...	2.134	13.7	ng	910126	1	6.816	1329630	20.0
2-Pentanone, 4-...	5.034	21.4	ng	1420530	1	6.816	1329630	20.0
2-Pentanone, 4-...	5.828	2.3	ng	149869	1	6.816	1329630	20.0
Hexadecanoic ac...	11.739	2.4	ng	231823	4	11.339	1952630	20.0
n-Hexadecanoic ...	11.868	2.6	ng	257145	4	11.339	1952630	20.0
1-Heneicosanol	13.851	14.1	ng	1196770	5	13.974	1695410	20.0
Squalene	14.833	6.3	ng	450887	6	15.421	1426530	20.0
1-Heptacosanol	16.009	3.1	ng	221166	6	15.421	1426530	20.0