LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082925\
Data File : BP025622.D
Acq On : 29 Aug 2025 12:36
Operator : CG/JU
Sample : Q2971-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP2

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\8270E-BP081425.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP025622.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.025	10	15	20	rBV	1280763	1643365	14.60%	2.196%
2	4.931	332	339	346	rBV	479811	690574	6.14%	0.923%
3	5.396	409	418	429	rBV	3642587	5610371	49.85%	7.498%
4	6.966	677	685	695	rBV	3506716	5785658	51.41%	7.732%
5	7.766	814	821	829	rVB	702431	1144726	10.17%	1.530%
6	8.913	1008	1016	1029	rVB	2285372	3854422	34.25%	5.151%
7	10.537	1285	1292	1301	rBV	952664	1551519	13.79%	2.074%
8	12.995	1702	1710	1721	rBV	5064077	7996257	71.05%	10.687%
9	14.384	1940	1946	1953	rBV	1257105	1953257	17.36%	2.610%
10	15.760	2175	2180	2186	rBV2	434244	744834	6.62%	0.995%
11	15.895	2198	2203	2211	rVB	4615111	6532354	58.05%	8.730%
12	16.560	2311	2316	2330	rVB9	229317	695351	6.18%	0.929%
13	17.178	2416	2421	2427	rBV	1718118	2533265	22.51%	3.386%
14	17.242	2429	2432	2436	rVB3	79225	119728	1.06%	0.160%
15	18.119	2575	2581	2592	rBV	2784399	4030826	35.82%	5.387%
16	18.442	2633	2636	2642	rVB	288571	393160	3.49%	0.525%
17	18.801	2694	2697	2704	rVB4	157353	272607	2.42%	0.364%
18	18.889	2709	2712	2717	rVB	170840	223014	1.98%	0.298%
19	19.266	2770	2776	2783	rBV	644717	1204227	10.70%	1.609%
20	19.442	2802	2806	2815	rBV	869362	1264214	11.23%	1.690%
21	19.901	2878	2884	2889	rVB	8508417	11253801	100.00%	15.040%
22	19.954	2891	2893	2902	rVB2	158409	288380	2.56%	0.385%
23	20.207	2933	2936	2940	rVB2	258508	324947	2.89%	0.434%
24	21.154	3090	3097	3104	rBV	2867299	4907698	43.61%	6.559%
25	21.283	3115	3119	3124	rBV	891763	1405681	12.49%	1.879%
26	21.477	3147	3152	3166	rBV2	812900	2568368	22.82%	3.433%
27	21.624	3173	3177	3183	rVB	1679903	2650339	23.55%	3.542%
28	24.995	3746	3750	3764	rVB	1099699	3181486	28.27%	4.252%

Sum of corrected areas: 74824429

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082925\
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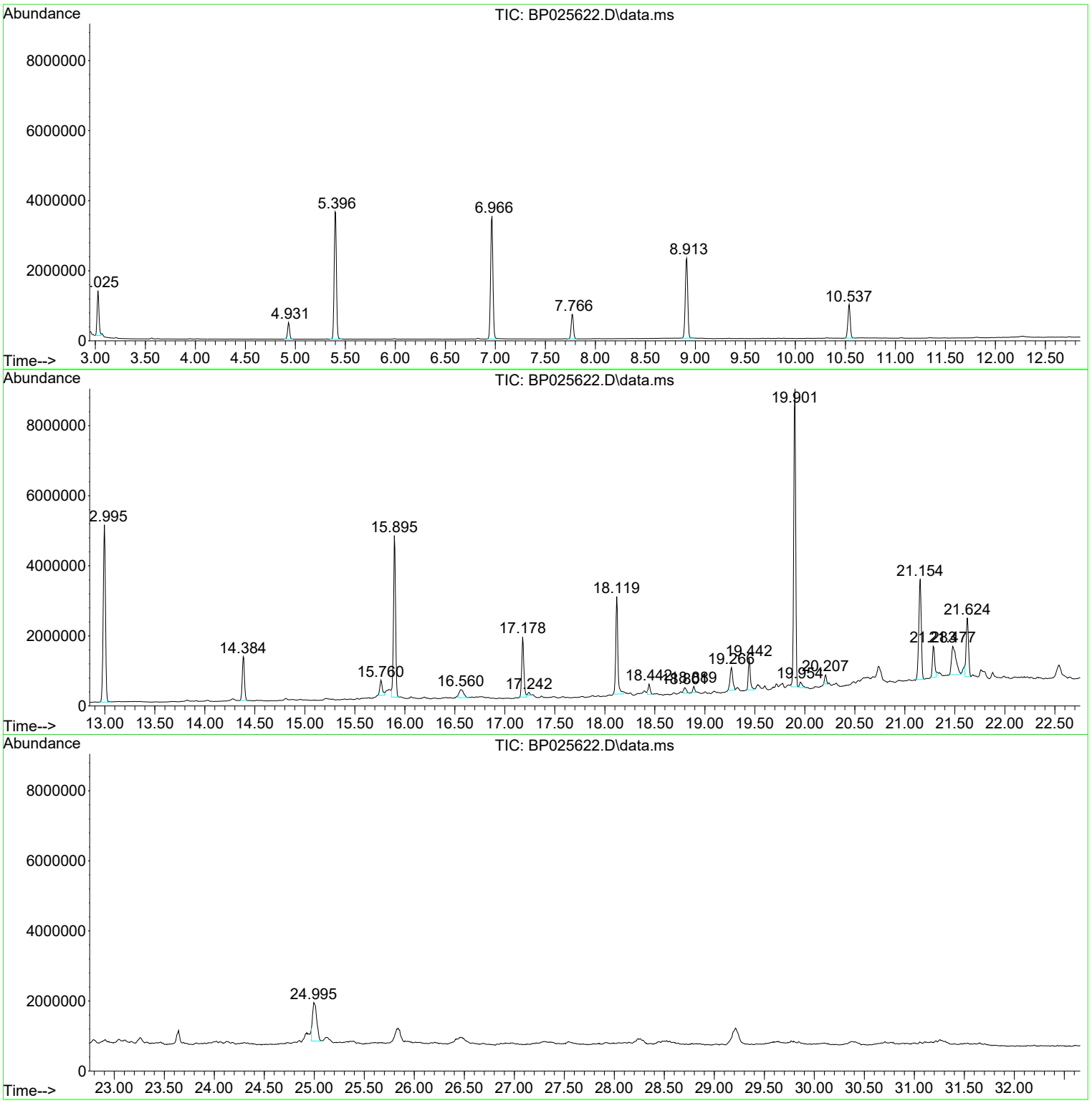
Sample : Q2971-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.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_P\Data\BP082925\
Data File : BP025622.D
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Operator : CG/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

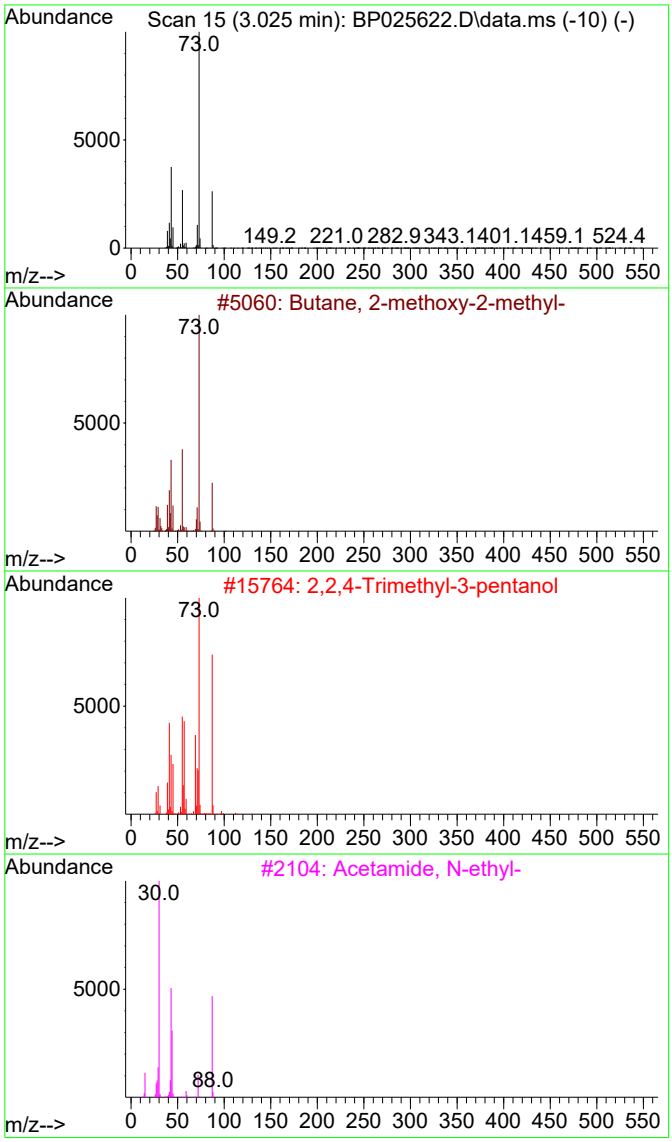
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

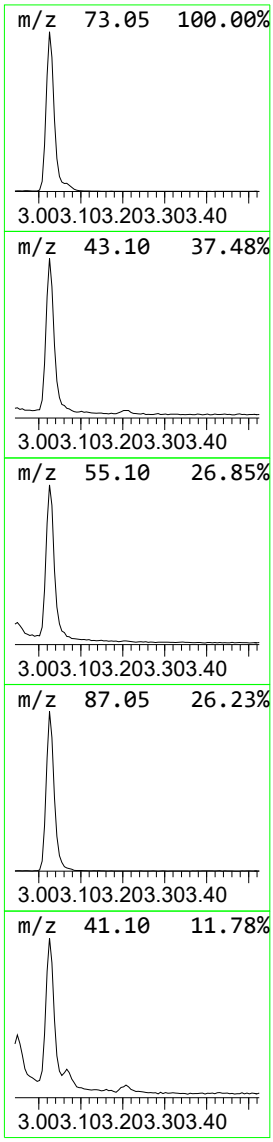
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.025	28.71 ng	1643370	1,4-Dichlorobenzene-d4	7.772

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Data File : BP025622.D
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ALS Vial : 4 Sample Multiplier: 1

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ClientSampleId :
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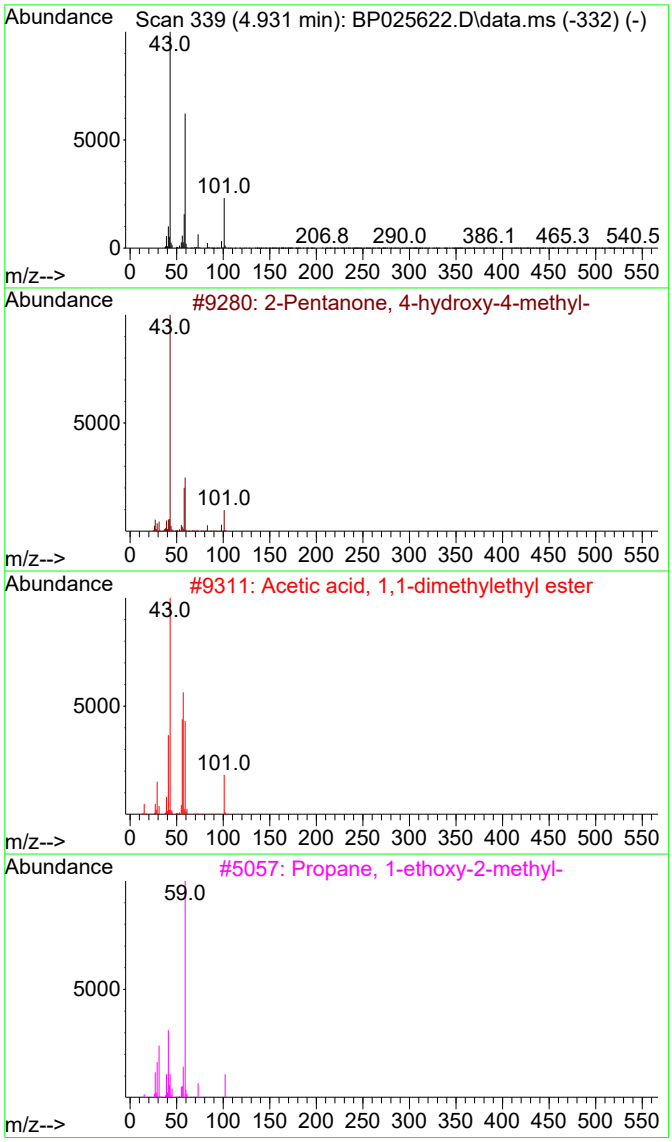
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

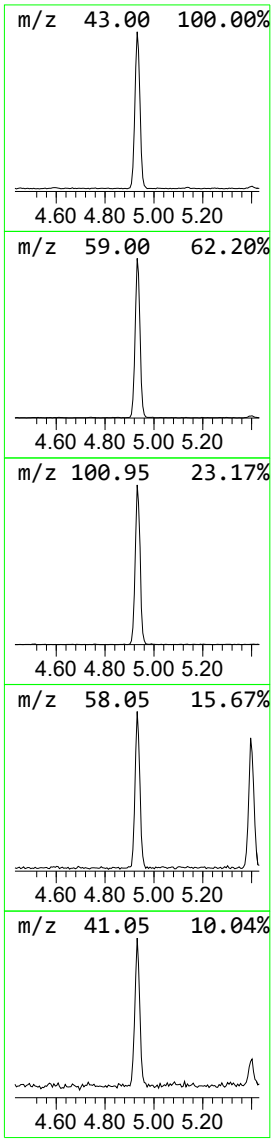
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.931	12.07 ng	690574	1,4-Dichlorobenzene-d4	7.772

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	17





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Operator : CG/JU
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
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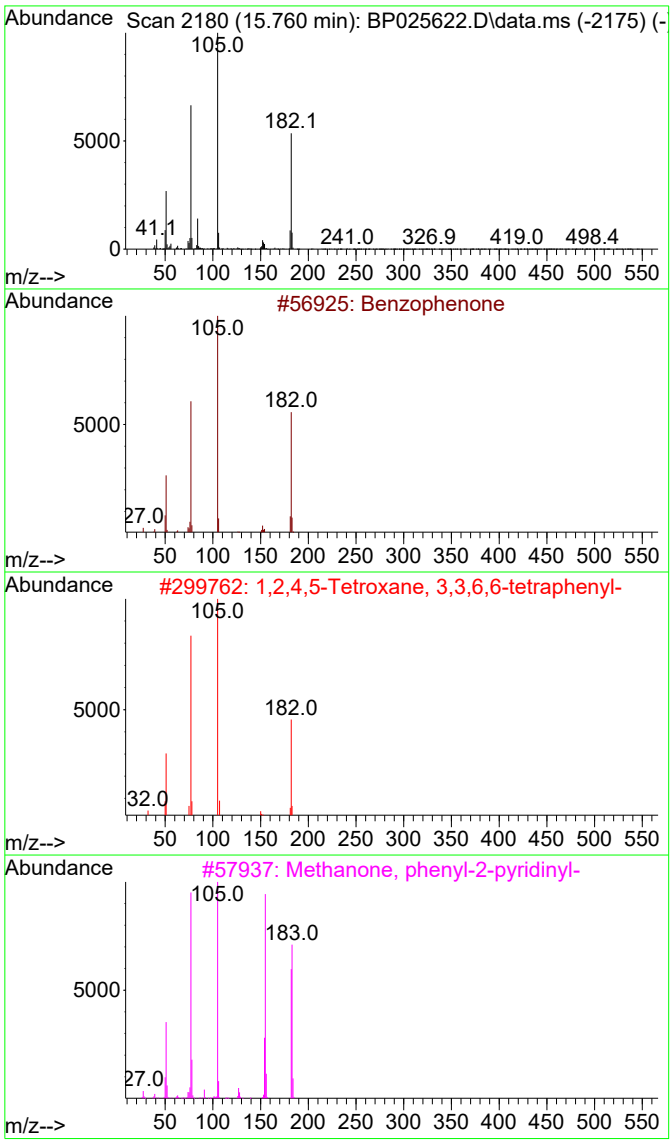
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

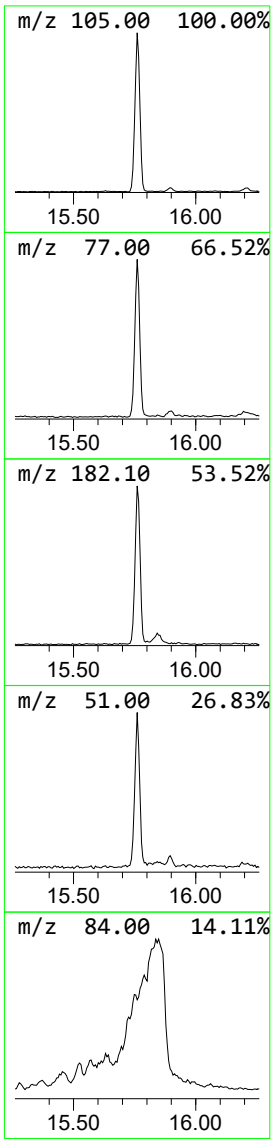
****

Peak Number 3 Benzophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.760	7.63 ng	744834	Acenaphthene-d10	14.384

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	72
3	Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	50
4	Azobenzene, (E)-	182	C12H10N2	017082-12-1	42
5	Azobenzene	182	C12H10N2	000103-33-3	37





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
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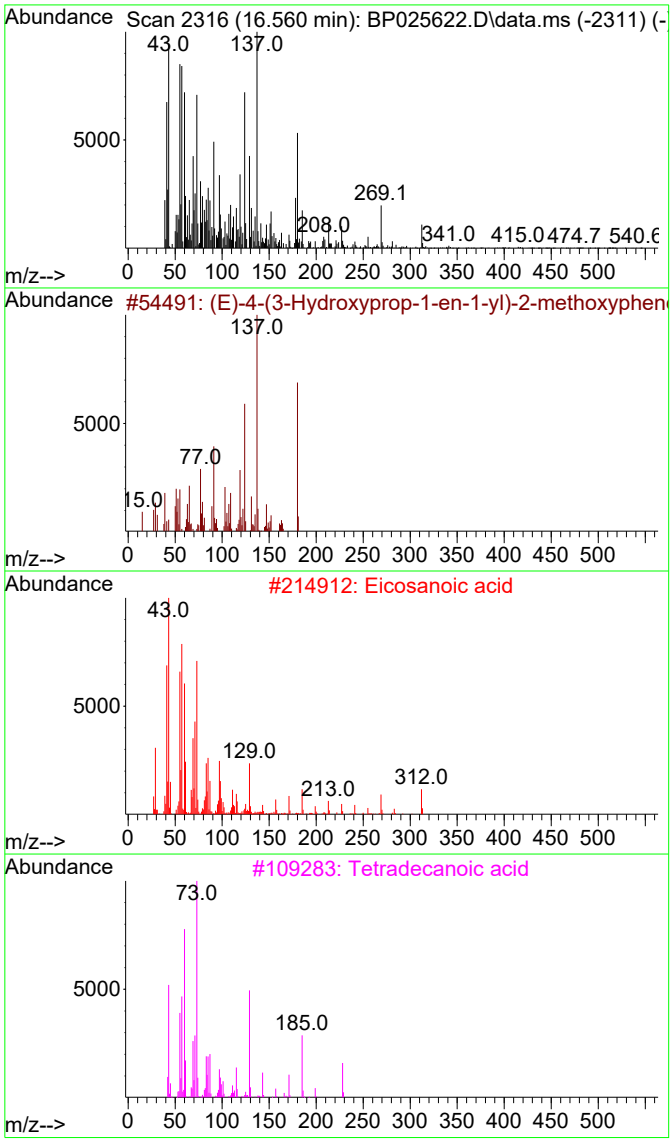
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

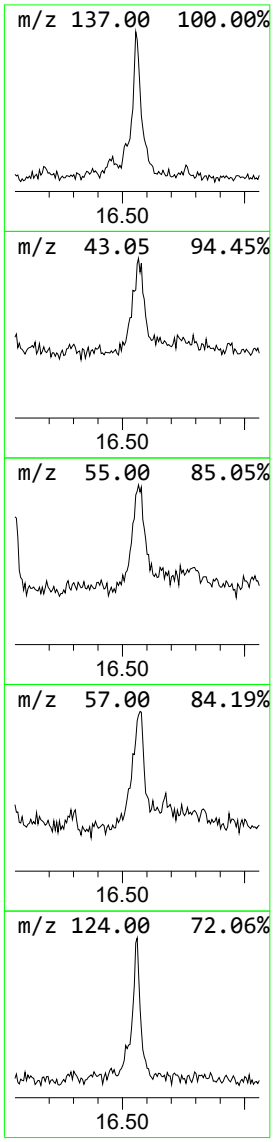
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (E)-4-(3-Hydroxyprop-1-en-1... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.560	5.49 ng	695351	Phenanthrene-d10	17.178

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-4-(3-Hydroxyprop-1-en-1-yl)-...	180	C10H12O3	032811-40-8	53
2	Eicosanoic acid	312	C20H40O2	000506-30-9	41
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	25
4	Benzene, 1-methyl-4-[(2-methylpr...	180	C11H16S	054576-37-3	25
5	Benzene, 1-methyl-3-[(2-methylpr...	180	C11H16S	054576-36-2	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082925\
Data File : BP025622.D
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Operator : CG/JU
Sample : Q2971-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

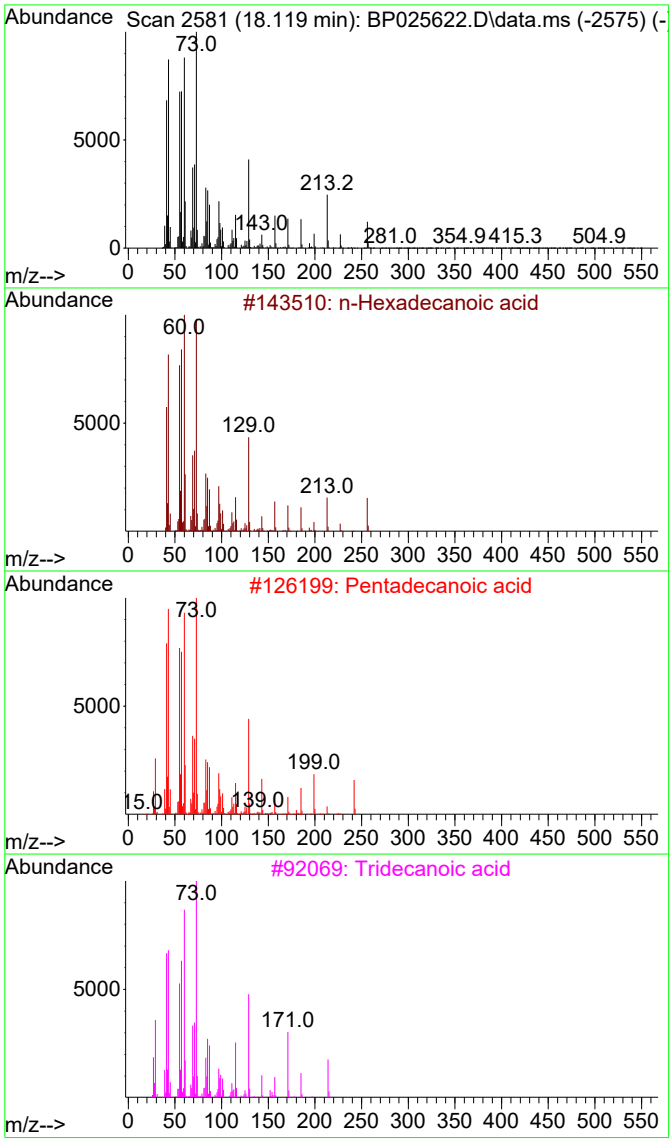
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

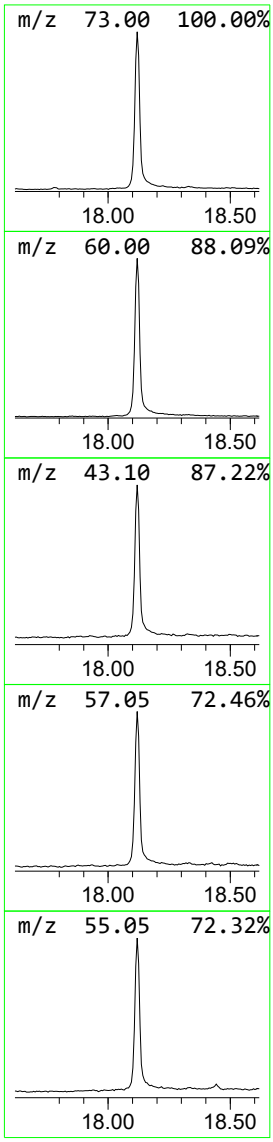
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.119	31.82 ng	4030830	Phenanthrene-d10	17.178

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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	76





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Sample : Q2971-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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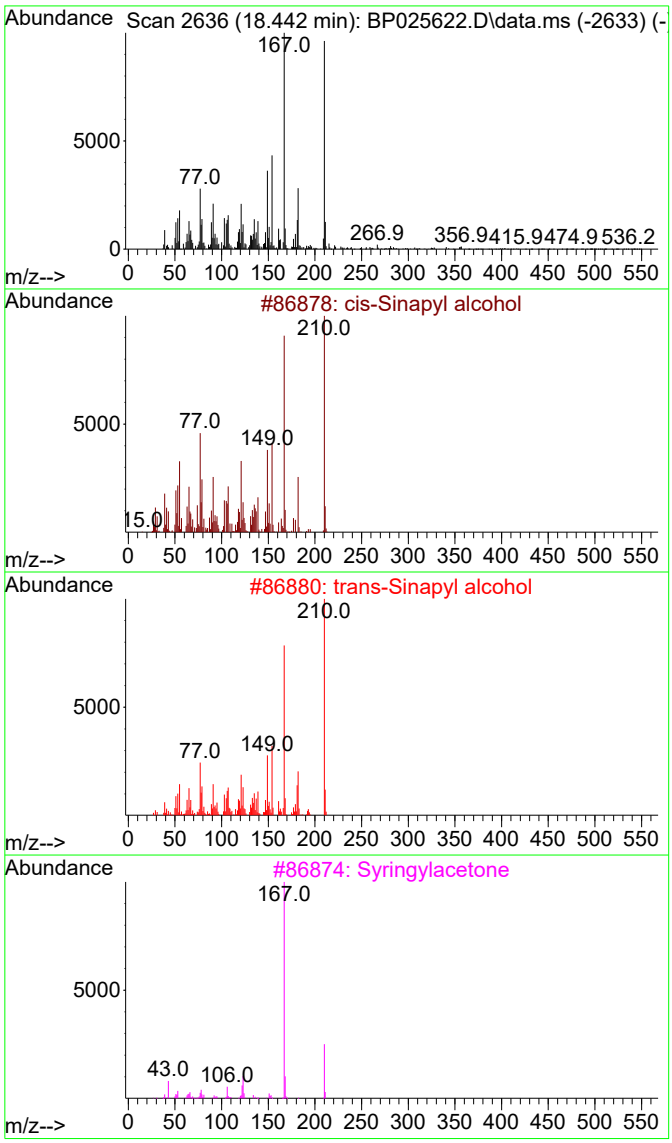
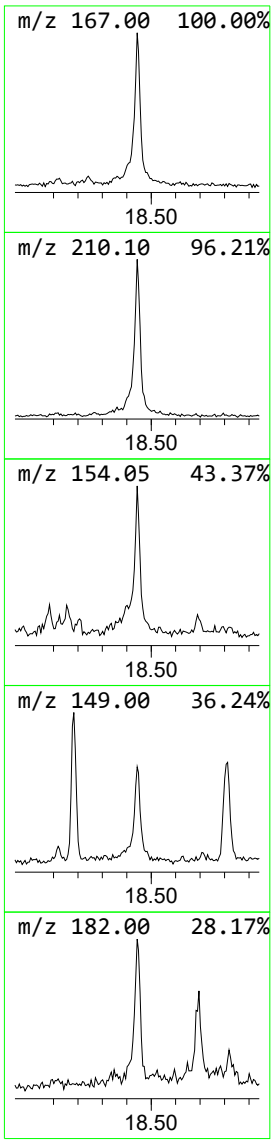
****

Peak Number 6 cis-Sinapyl alcohol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.442	3.10 ng	393160	Phenanthrene-d10	17.178

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	94
2	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	93
3	Syringylacetone	210	C11H14O4	019037-58-2	53
4	1-Butyl-6,7-difluoro-1,3-benzimi...	210	C11H12F2N2	1375069-34-3	50
5	4-Ethoxy-2,5-dimethoxybenzaldehyde	210	C11H14O4	1000121-30-2	46





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Data File : BP025622.D
Acq On : 29 Aug 2025 12:36
Operator : CG/JU
Sample : Q2971-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

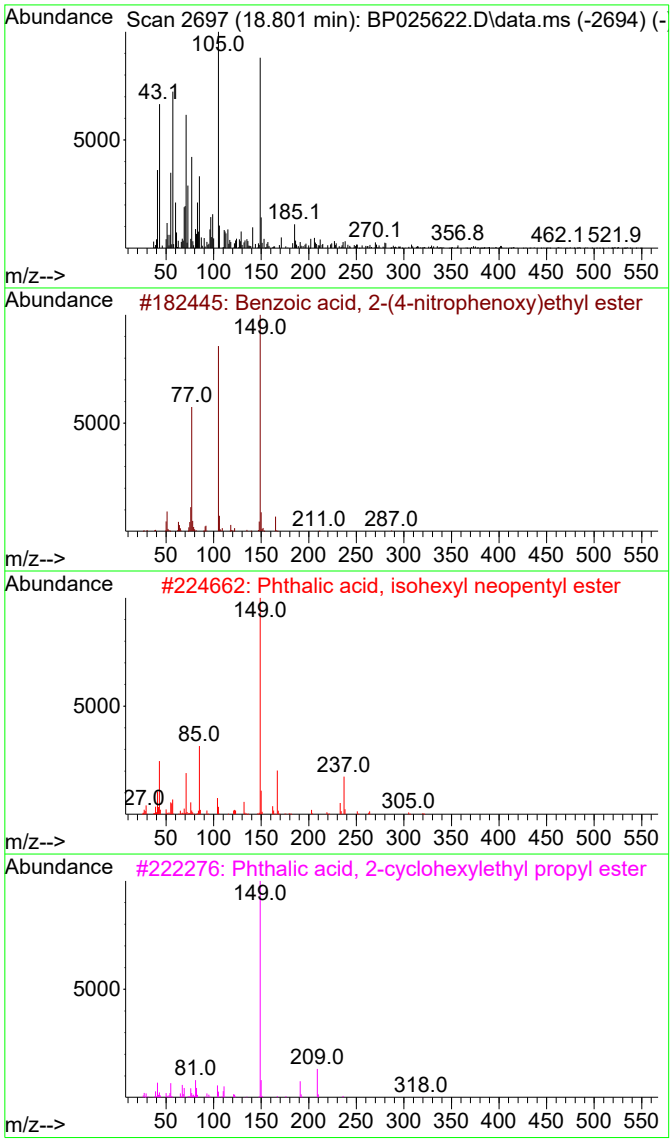
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

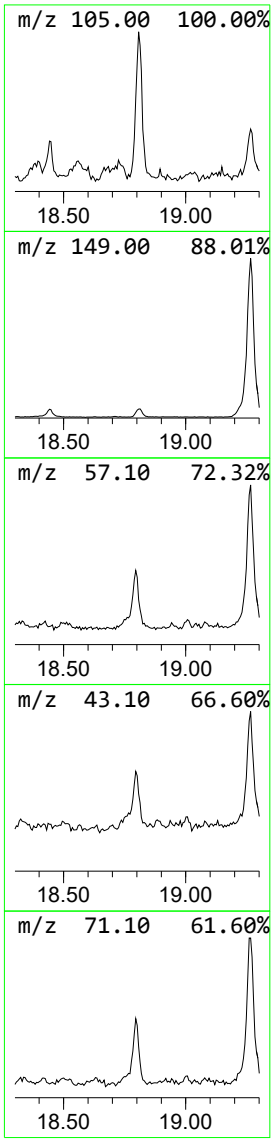
****

Peak Number 7 unknown18.801 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.801	2.15 ng	272607	Phenanthrene-d10	17.178

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	43
2	Phthalic acid, isohexyl neopenty...	320	C19H28O4	1000308-97-7	41
3	Phthalic acid, 2-cyclohexylethyl...	318	C19H26O4	1000309-08-5	30
4	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	25
5	Phthalic acid, isoporpyl pentyl ...	278	C16H22O4	1000314-99-9	25





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TIC Library : C:\Database\NIST20.L
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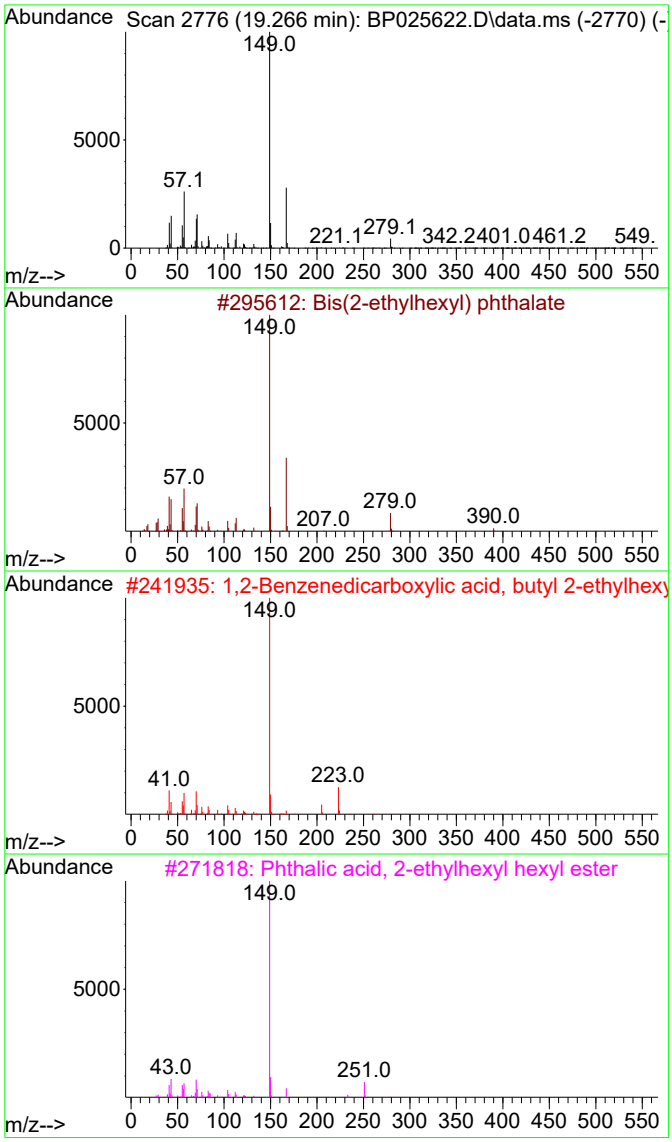
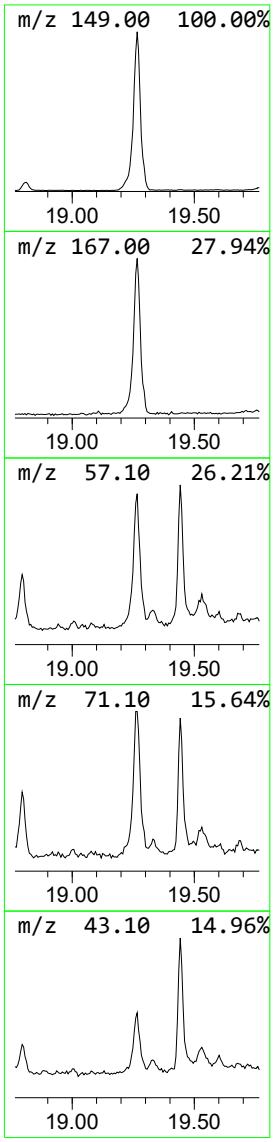
****
Peak Number 8 1,2-Benzenedicarboxylic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.266	9.51 ng	1204230	Phenanthrene-d10	17.178

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	91
2	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	72
3	Phthalic acid, 2-ethylhexyl hexy...	362	C22H34O4	1000309-02-5	72
4	Phthalic acid, hept-4-yl isohexy...	348	C21H32O4	1000356-78-6	72
5	Phthalic acid, di(hex-3-yl) ester	334	C20H30O4	1000356-96-7	64





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ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

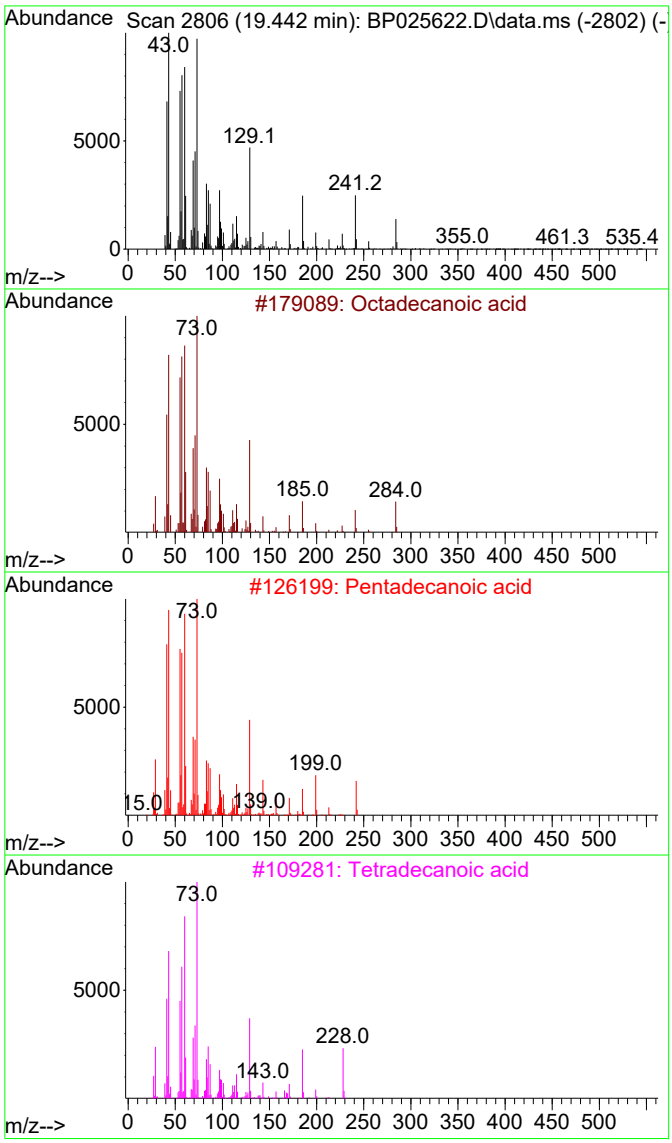
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

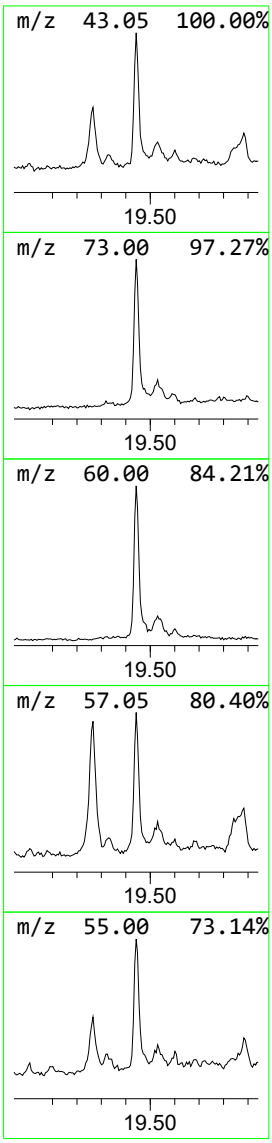
****

Peak Number 9 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.442	9.54 ng	1264210	Chrysene-d12	21.624

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





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ClientSampleId :
TP2

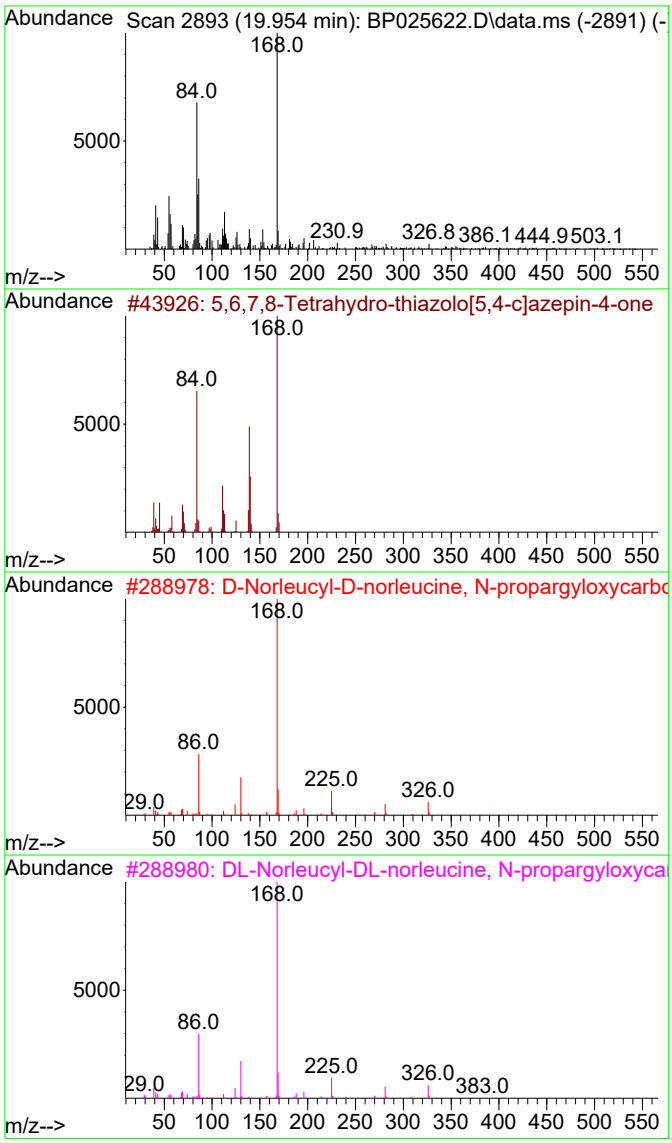
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

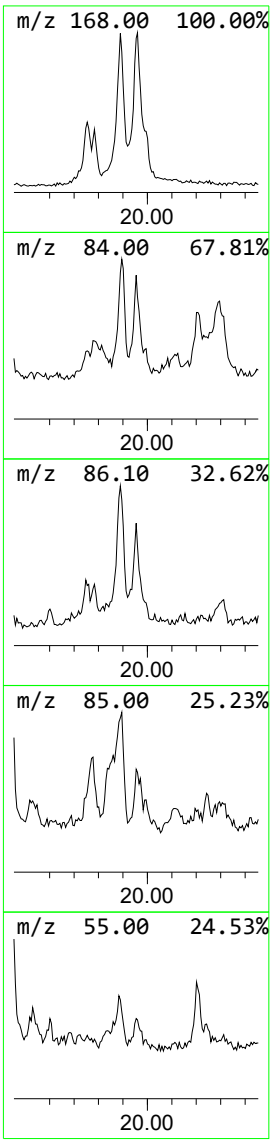
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 5,6,7,8-Tetrahydro-thiazolo... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.954	2.18 ng	288380	Chrysene-d12	21.624

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,6,7,8-Tetrahydro-thiazolo[5,4-...	168	C7H8N2OS	1000317-75-4	59
2	D-Norleucyl-D-norleucine, N-prop...	382	C20H34N2O5	1000344-23-8	46
3	DL-Norleucyl-DL-norleucine, N-pr...	382	C20H34N2O5	1000344-08-4	46
4	4-Methoxy-2,2,5-trimethylcyclope...	168	C9H12O3	1000185-67-3	38
5	6-Chloro-1,3-benzoxazol-2-amine	168	C7H5ClN2O	052112-68-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082925\
Data File : BP025622.D
Acq On : 29 Aug 2025 12:36
Operator : CG/JU
Sample : Q2971-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

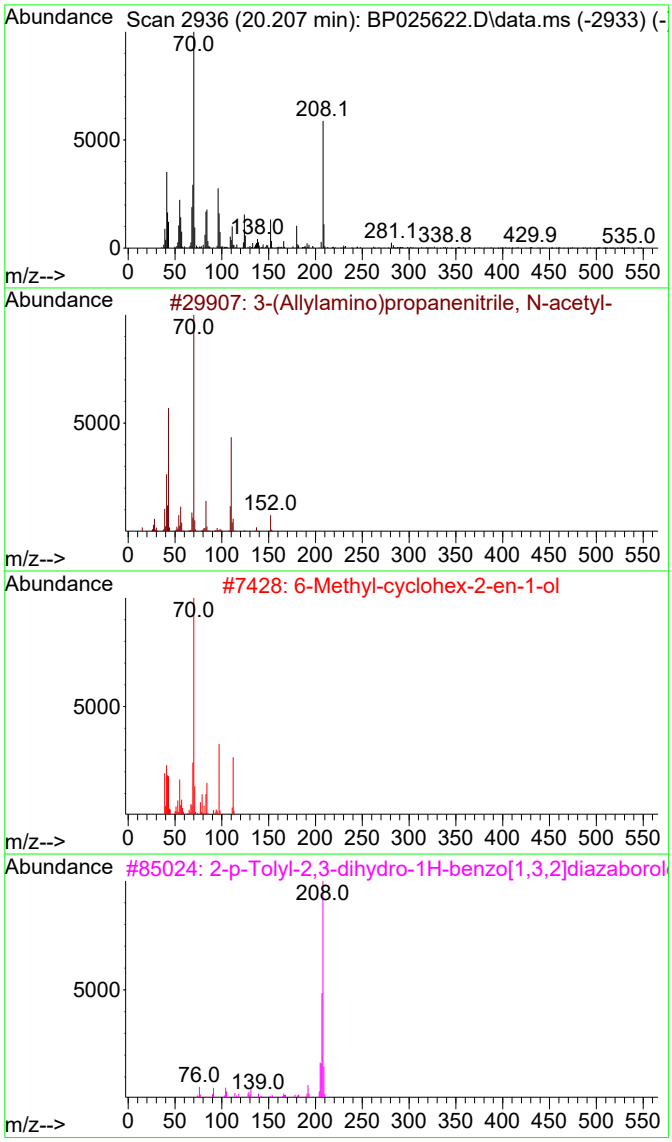
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

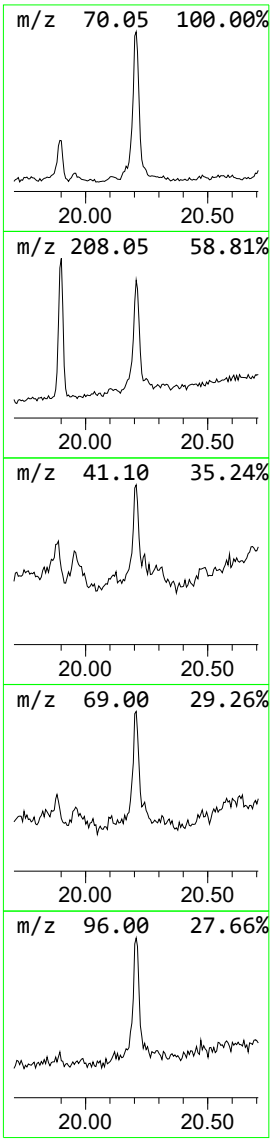
****

Peak Number 11 unknown20.207 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.207	2.45 ng	324947	Chrysene-d12	21.624

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(Allylamino)propanenitrile, N-...	152	C8H12N2O	1000475-61-4	38
2	6-Methyl-cyclohex-2-en-1-ol	112	C7H12O	1000144-17-3	35
3	2-p-Tolyl-2,3-dihydro-1H-benzo[1...	208	C13H13BN2	1000296-11-8	27
4	2,3-Dimethyl-1-hexene	112	C8H16	016746-86-4	27
5	3-(Cyclopropylamino)propionitrile	110	C6H10N2	058196-47-7	27





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Data File : BP025622.D
Acq On : 29 Aug 2025 12:36
Operator : CG/JU
Sample : Q2971-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP2

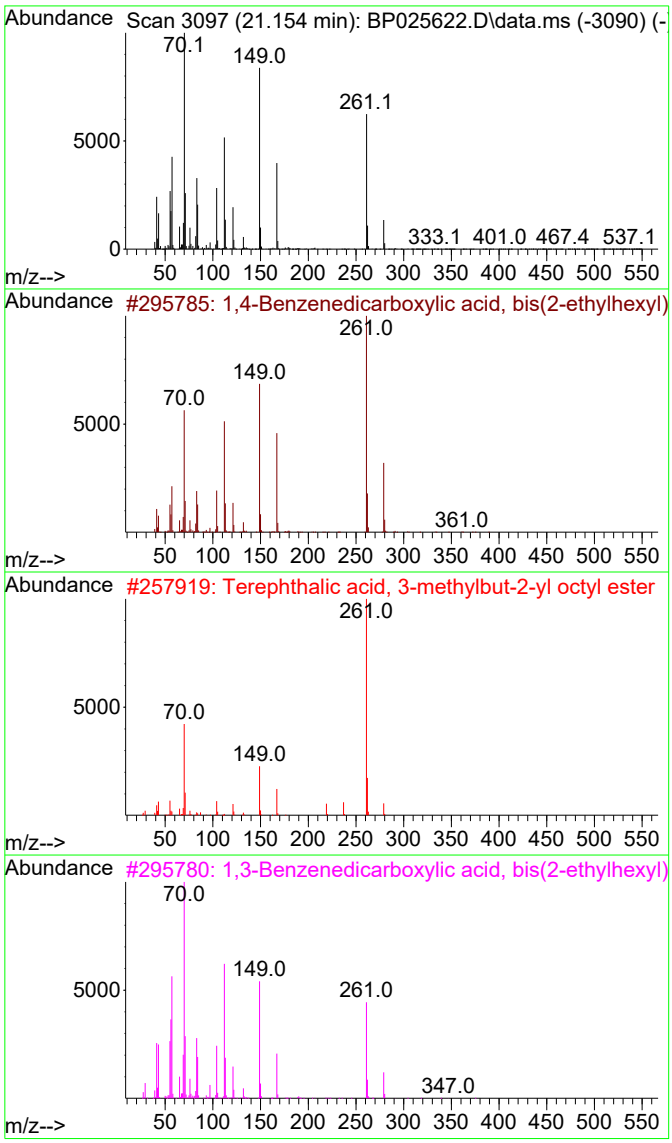
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

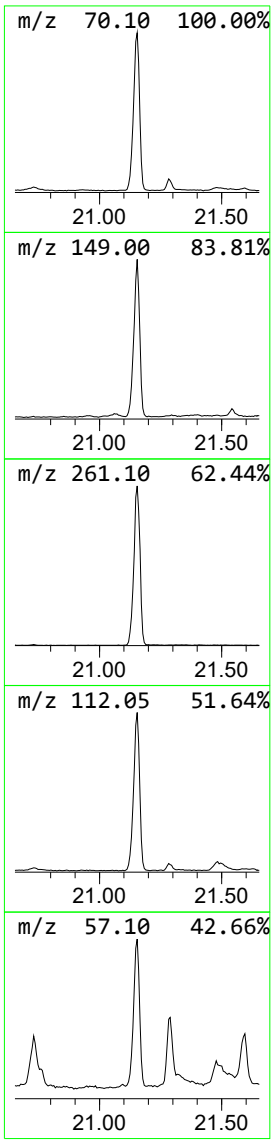
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 1,4-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.154	37.03 ng	4907700	Chrysene-d12	21.624

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	87
2	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	64
3	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	62
4	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	43
5	Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43





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Operator : CG/JU
Sample : Q2971-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.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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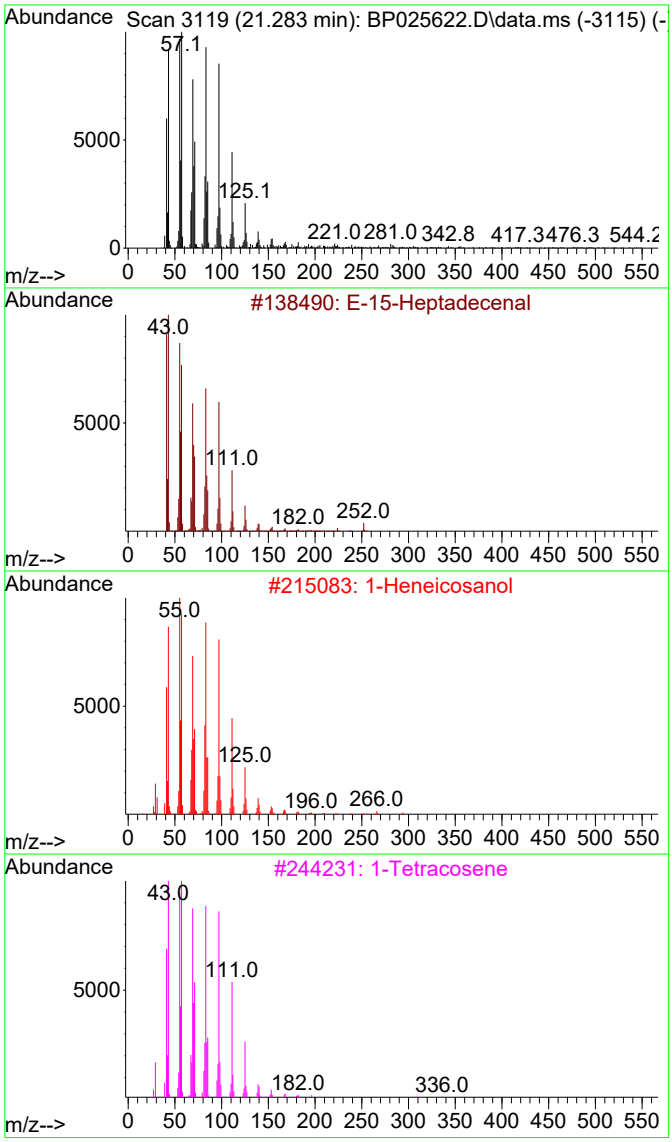
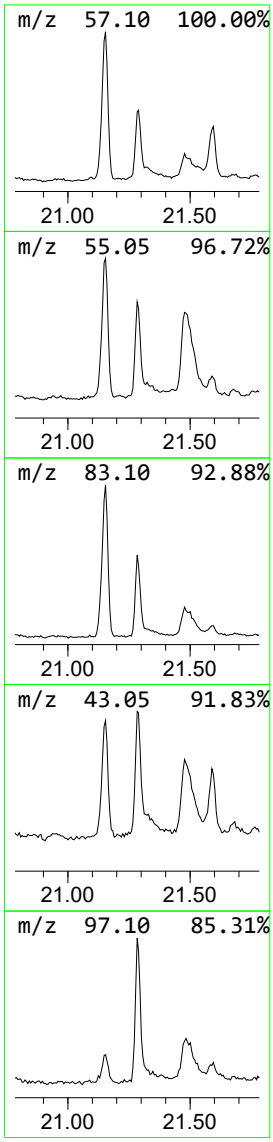
Peak Number 13 E-15-Heptadecenal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.283	10.61 ng	1405680	Chrysene-d12	21.624

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	97
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	1-Tetracosene	336	C24H48	010192-32-2	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	1-Tricosene	322	C23H46	018835-32-0	94





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Operator : CG/JU
Sample : Q2971-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

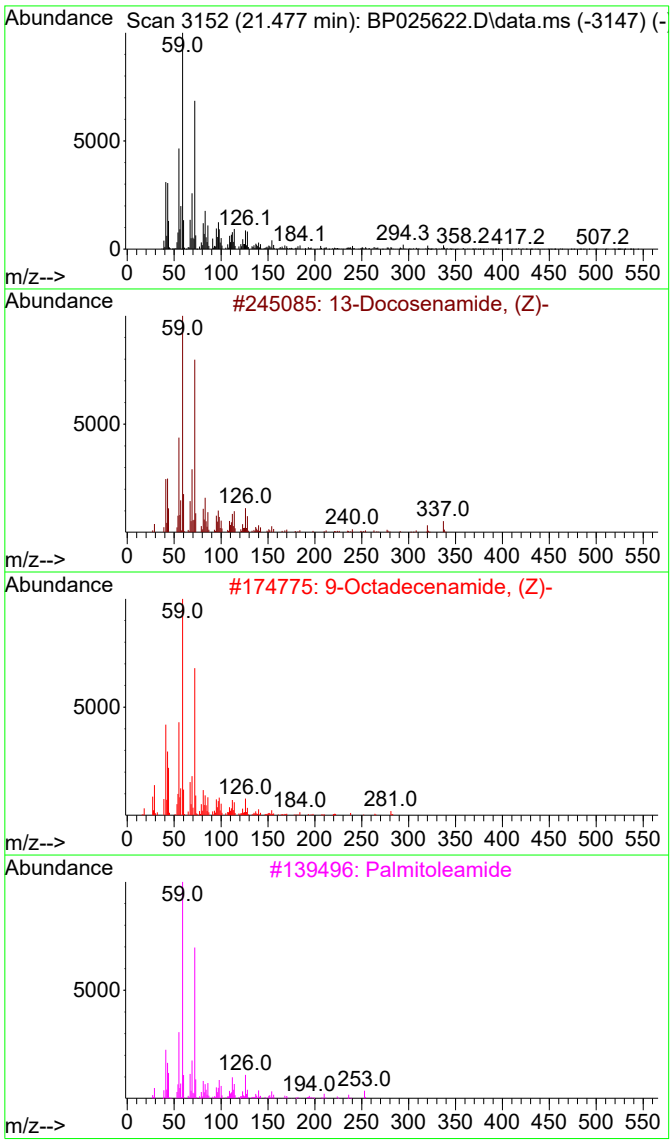
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

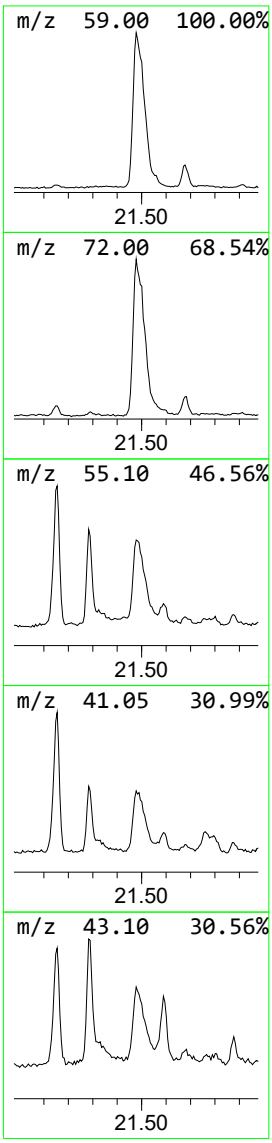
****

Peak Number 14 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.477	19.38 ng	2568370	Chrysene-d12	21.624

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	98
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
3	Palmitoleamide	253	C16H31NO	106010-22-4	72
4	Hexadecanamide	255	C16H33NO	000629-54-9	64
5	Octadecanamide	283	C18H37NO	000124-26-5	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082925\
Data File : BP025622.D
Acq On : 29 Aug 2025 12:36
Operator : CG/JU
Sample : Q2971-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.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...	3.025	28.7	ng	1643370	1	7.772	1144730	20.0
2-Pentanone, 4-...	4.931	12.1	ng	690574	1	7.772	1144730	20.0
Benzophenone	15.760	7.6	ng	744834	3	14.384	1953260	20.0
(E)-4-(3-Hydrox...	16.560	5.5	ng	695351	4	17.178	2533270	20.0
n-Hexadecanoic ...	18.119	31.8	ng	4030830	4	17.178	2533270	20.0
cis-Sinapyl alc...	18.442	3.1	ng	393160	4	17.178	2533270	20.0
unknown18.801	18.801	2.1	ng	272607	4	17.178	2533270	20.0
1,2-Benzenedica...	19.266	9.5	ng	1204230	4	17.178	2533270	20.0
Octadecanoic acid	19.442	9.5	ng	1264210	5	21.624	2650340	20.0
5,6,7,8-Tetrahy...	19.954	2.2	ng	288380	5	21.624	2650340	20.0
unknown20.207	20.207	2.5	ng	324947	5	21.624	2650340	20.0
1,4-Benzenedica...	21.154	37.0	ng	4907700	5	21.624	2650340	20.0
E-15-Heptadecenal	21.283	10.6	ng	1405680	5	21.624	2650340	20.0
13-Docosenamide...	21.477	19.4	ng	2568370	5	21.624	2650340	20.0